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Chemical Physics Letters 211–220 (1994) 1–103

CHEMICAL PHYSICS LETTERS

Master index to volumes 211–220

Abdelaoui, O., see L. Schriver-Mazzuoli 214 (1993) 519
Abdel-Latif, F.M., see T. Nakayama 220 (1994) 219
Åberg, U., E. Åkesson and V. Sundström, Excited state dynamics of barrierless isomerization in solution 215 (1993) 388
Abner, D., see J. Holtgrave 215 (1993) 548
Abouaf, R., J. Pommier and S. Cvejanovic, Electron impact on free C_{60}. Excited states below 10 eV 213 (1993) 503
Abresch, E.C., see A. Van der Est 212 (1993) 561
Achiba, Y., see F. Negri 211 (1993) 353
Achiba, Y., see K. Kikuchi 216 (1993) 67
Achiwa, N., see K. Mukai 214 (1993) 559
Ackermann, J. and R. Roitzsch, A two-dimensional multilevel adaptive finite element method for the time-independent Schrödinger equation 214 (1993) 109
Acuña, A.U., see A. Douhal 217 (1994) 619
Adachi, H., see T. Mukoyama 215 (1993) 93
Adachi, H., see J. Onoe 217 (1994) 61
Adam, P., see J. Janszky 213 (1993) 368
Adamčíková, L., see I. Valent 216 (1993) 479
Adamo, C., see V. Barone 212 (1993) 5
Adamowicz, L., see N.A. Oyler 219 (1994) 223
Adhikari, S., see P. Dutta 212 (1993) 677
Aegerter, M.A., see S.J.L. Ribeiro 220 (1994) 214
Afzaal, S. and B.S. Freiser, Gas-phase photodissociation study of Ag(benzene)$^+$ and Ag(toluene) 218 (1994) 254
Agafonov, V., see B. Keita 215 (1993) 125
Ågren, H., see Y. Luo 213 (1993) 356
Ågren, H., see B. Minaev 217 (1994) 531
Agterberg, D.F., W. Que and M.B. Walker, Comment on "Structure and lattice dynamics of the ordered phase of solid C_{70}" 213 (1993) 207
Aguilar, A., M. Albertí, J. de Andrés, M. Gilibert, X. Giménez, M. González, J.M. Lucas, M. Prieto, R. Sayós and A. Solé, Crossed molecular beams study of the $M^+(^1S)+Na(3\,^2S)\rightarrow M^+(^1S)+Na(3\,^2P)$ collision systems ($M^+=Li^+$, Na^+, K^+, Cs^+) in the 0.05–3.00 keV energy range 220 (1994) 267
Ahn, J.S., Y. Kanematsu, M. Enomoto and T. Kushida, Determination of weighted density of states of vibrational modes in Zn-substituted myoglobin 215 (1993) 336
Ajayan, P.M., J.M. Lambert, P. Bernier, L. Barbedette, C. Colliex and J.M. Planeix, Growth morphologies during cobalt-catalyzed single-shell carbon nanotube synthesis 215 (1993) 509
Ajello, J.M., see I. Kanik 211 (1993) 523

Åkesson, E., see U. Åberg 215 (1993) 388
Aksela, H., see O.-P. Sairanen 215 (1993) 353
Aksela, S., see O.-P. Sairanen 215 (1993) 353
Akselrod, L., H.J. Byrne, C. Thomsen, A. Mittelbach and S. Roth, Raman studies of photochemical reactions in fullerene films 212 (1993) 384
Akselrod, L., see K. Kamarás 214 (1993) 338
Akselrod, L., H.J. Byrne, C. Thomsen and S. Roth, Reversible photochemical processes in fullerenes. A Raman study 215 (1993) 131
Albertí, M., see A. Aguilar 220 (1994) 267
Albrecht, A.C., see S.K. Lim 216 (1993) 405
Alcalá, R., see E. Bayer 216 (1993) 228
Aleksandrov, N.L., Three-body electron attachment to $O_2(a\ ^1\Delta_g)$ 212 (1993) 409
Alekseyev, A.B., see H.-P. Liebermann 214 (1993) 381
Alexandrov, V.I., A.V. Zaitsevskii and A.I. Dement'ev, Modified Padé approximation scheme to resume the intermediate Hamiltonian QDPT series 218 (1994) 206
Alfè, D., P. Rudolf, M. Kiskinova and R. Rosei, HREEL spectra of various oxygen structures on Rh(110) 211 (1993) 220
Al-Hassan, K.A., U.K.A. Klein and A. Suwaiyan, Normal and twisted intramolecular charge-transfer fluorescence of 4-dimethylaminobenzonitrile in α-cyclodextrine cavities 212 (1993) 581
Al-Kahali, M.S.N., R.J. Donovan, K.P. Lawley and T. Ridley, Sequential two-photon excitation via repulsive intermediate states 220 (1994) 225
Allman, S.L., see R.B. Jones 212 (1993) 451
Almlöf, J., see O. Vahtras 213 (1993) 514
Almlöf, J., see A. Ghosh 213 (1993) 519
Almlöf, J., see Y.C. Zheng 214 (1993) 397
Al-Omari, A. and R. Reininger, Electric field effects in the photoionization and photoabsorption of methyl iodide 220 (1994) 437
Alsanoosi, A.M., see S. Clough 211 (1993) 637
Altibelli, A., see C. Chavy 214 (1993) 569; 219 (1994) 502
Altmann, R.B., D. Haarer and I. Renge, Stark effect on spectral holes of chlorophyll a at 2 K 216 (1993) 281
Amat-Guerri, F., see A. Douhal 217 (1994) 619
Amosov, K.A., see S.A. Nizkorodov 215 (1993) 662
Amstrup, B., see N.E. Henriksen 213 (1993) 65
Ananthavel, S.P., B. Ganguly, J. Chandrasekhar, M.S. Hegde and C.N.R. Rao, Electron states of benzene...HCl and toluene...HCl hydrogen bonded complexes by ultraviolet photoelectron spectroscopy 217 (1994) 101
Andersen, L.H., C. Brink, H.K. Haugen, P. Hvelplund, D.H. Yu, N. Hertel and S.P. Møller, Lifetime measurements with fullerene ions in a heavy-ion storage ring 217 (1994) 204
Andersson, S., see P.A. Brühwiler 214 (1993) 45
Andrae, D., M. Dolg, H. Stoll and W.C. Ermler, Comment on "Comparison of the widely used HF pseudo-potentials: MH^+ (M=Fe, Ru, Os)" 220 (1994) 341
André, D., see B. Keita 215 (1993) 125
André, J.C., see A.T. Reis e Sousa 213 (1993) 333
Andreoni, W., see G. Onida 219 (1994) 1
Andzelm, J., see J. Baker 216 (1993) 380
Angerhofer, A., see G.G. Lazarev 215 (1993) 375

Angerhofer, A., J.U. von Schütz, D. Widmann, W.H. Müller, H.U. ter Meer and H. Sixl, The triplet state of C_{60} studied by zero-field absorption-detected magnetic resonance 217 (1994) 403
Ángyán, J.G., G. Jansen, M. Loos, C. Hättig and B.A. Heß, Distributed polarizabilities using the topological theory of atoms in molecules 219 (1994) 267
Aoiz, F.J., V.J. Herrero, M.M. Nogueira and V. Sáez Rábanos, Quasiclassical trajectory study of a two ends reaction: F+HD→HF (DF)+D (H). Comparison of vibrationally state-resolved integral and differential cross sections on three different surfaces 211 (1993) 72
Aoiz, F.J., L. Bañares, V.J. Herrero and V. Sáez Rábanos, Classical dynamics calculations for the $F+H_2 \rightarrow HF+H$ reaction on two recent potential energy surfaces 218 (1994) 422
Aoki, H., see K. Okahara 219 (1994) 462
Aono, S., see H. Nagao 215 (1993) 5
Apkarian, V.A., see R. Zadoyan 218 (1994) 504
Arai, J., see T. Miyazaki 219 (1994) 405
Arai, T., Y. Furuya, H. Furuuchi and K. Tokumaru, One-way Z→E isomerization around the double bond of N-methoxy-1-(2-anthryl)ethanimine in the excited triplet state. Direct observation of one-way isomerization from Z triplet to E triplet of the C=N bond 212 (1993) 597
Aratono, Y., see Y. Fujitani 214 (1993) 301
Arratia-Pérez, R., The $M_6S_8L_6$ clusters: an example in cluster and condensed phase chemistry 213 (1993) 547
Aruga, T., see T. Takaoka 215 (1993) 523
Arusi-Parpar, T., see S. Koppe 214 (1993) 546
Arvanitis, D., G. Comelli, T. Lederer, H. Rabus and K. Baberschke, Characterization of two different adsorption states for O on Cu(100). Ionic versus covalent bonding 211 (1993) 53
Asaf, U., S. Felps, K. Rupnik and S.P. McGlynn, A pressure-shift study of electron scattering in dense hydrogen–argon gas mixtures 212 (1993) 326
Ashfold, M.N.R., see M.D. Wheeler 211 (1993) 381
Ashjian, P., see R. Zadoyan 218 (1994) 504
Astaldi, C., see C. Comicioli 214 (1993) 438
Asthana, B.P., see R.K. Singh 213 (1993) 210
Astilean, S., V. Chitta, A. Corval, R.J.D. Miller and H.P. Trommsdorff, Singlet–triplet level crossings in matrix-isolated pentacene 219 (1994) 95
Ataev, M., see B.Z. Gorbunov 215 (1993) 31
Athanassenas, K., D. Kreisle, B.A. Collings, D.M. Rayner and P.A. Hackett, Ionization potentials of niobium cluster oxides 213 (1993) 105
Atkinson, J.B., see J. Supronowicz 213 (1993) 282; 218 (1994) 240
Atkinson, J.B., see W. Kedzierski 215 (1993) 185; 218 (1994) 314
Atkinson, J.B., see J. Koperski 219 (1994) 161
Atrei, A., see C. Comicioli 214 (1993) 438
Augspurger, J.D., A.C. deDios, E. Oldfield and C.E. Dykstra, Computing nuclear magnetic resonance chemical shielding in large systems via multipole shielding polarizabilities 213 (1993) 211
Awadhesh Kumar, P.K. Chowdhury, K.V.S. Rama Rao and J.P. Mittal, IR and UV photolysis of 1,3-cyclohexadiene. Evidence for formation of vibrationally excited 1,3,5-hexatriene 212 (1993) 103
Azria, R., Y.L. Coat, J.-P. Ziesel, J.-P. Guillotin, B. Mharzi and M. Tronc, Mechanism for resonant O^- electron stimulated desorption from condensed O_2. Non-adiabatic transitions and dynamics 220 (1994) 417
Azuma, K., see S. Bachir 213 (1993) 54
Azumi, T., see T. Ikeyama 212 (1993) 551
Azumi, T., see H. Miki 218 (1994) 563

Baba, M., M. Brouard, S.P. Rayner and J.P. Simons, Elastic scattering dynamics of translationally and rotationally aligned molecular fragments via Doppler-resolved laser spectroscopy. OH($X\ ^2\Pi_{3/2}$) + Ar/He 220 (1994) 411
Babamov, V.K., Intramolecular hydrogen atom tunneling. Analytical solution for linear coupling to a low-frequency bath 217 (1994) 254
Baberschke, K., see D. Arvanitis 211 (1993) 53
Babić, D., D.J. Klein and C.H. Sah, Symmetry of fullerenes 211 (1993) 235
Babin, A., see S. Hess 216 (1993) 247
Bachilo, S.M. and T. Gillbro, Diphenyloctatetraene S_2 emission 218 (1994) 557
Bachir, S., J.C. Ronfard-Haret, K. Azuma, D. Kouyaté and J. Kossanyi, Direct impact excitation of thulium(III) luminescence in polycrystalline ZnO:Tm^{3+} electrodes in contact with an aqueous electrolyte, and attribution of the luminescence spectrum 213 (1993) 54
Bacis, R., see R. Stringat 220 (1994) 429
Bacsa, W.S., W.A. de Heer, D. Ugarte and A. Châtelain, Raman spectroscopy of closed-shell carbon particles 211 (1993) 346
Bacskay, G.B., see A.T. Wong 217 (1994) 17
Baer, M., see A. Baram 212 (1993) 649
Baer, M., H.-J. Loesch, H.-J. Werner and I. Last, Integral and differential cross sections for the Li + HF → LiF + H process. A comparison between j_z quantum mechanical and experimental results 219 (1994) 372
Bagratashvili, V.N., see S.M. Howdle 214 (1993) 215
Baguenard, B., see M. Pellarin 217 (1994) 349
Bai, J.-L., see Z.-L. Cai 220 (1994) 109
Baisogolov, A.Yu., see A.A. Buchachenko 220 (1994) 93
Bak, K.L., see M. Jaszunski 220 (1994) 154
Baker, J. and J.M. Dyke, A photoelectron and ab initio study of the CH_3SCH_2 radical 213 (1993) 257
Baker, J., S.K. Bramble and P.A. Hamilton, A hot band LIF study of the A $^1\Pi_u$–X $^1\Sigma_g^+$ transition in C_3 213 (1993) 297
Baker, J., V.C. Gibbons and P.A. Hamilton, Fourier transform optogalvanic spectroscopy 215 (1993) 163
Baker, J., A. Scheiner and J. Andzelm, Spin contamination in density functional theory 216 (1993) 380
Bakkas, N., see S. Coussan 217 (1994) 123
Bala, P., B. Lesyng and J.A. McCammon, Extended Hellmann–Feynman theorem for non-stationary states and its application in quantum-classical molecular dynamics simulations 219 (1994) 259
Balaban, A.T., D.J. Klein and C.A. Folden, Diamond–graphite hybrids 217 (1994) 266
Balaji, V., see H.S. Plitt 213 (1993) 158
Balasubramanian, K., see M. Benavides-Garcia 211 (1993) 631
Balasubramanian, K., Topological characterization of five C_{78} fullerene isomers (Chem. Phys. Letters 206 (1993) 210). Erratum 211 (1993) 649
Balasubramanian, K., see S. Roszak 212 (1993) 150; 215 (1993) 427
Balasubramanian, K., see D.-W. Liao 213 (1993) 174
Balasubramanian, K. and P.Y. Feng, Potential energy curves for electron beam excitation of $RbXe^+$ excimer 214 (1993) 85
Balasubramanian, K., see M. Vijayakumar 215 (1993) 87
Baldacchino, G., see P. Hébert 213 (1993) 345
Balková, A., see L. Meissner 212 (1993) 177
Ball, J.C., see T.J. Wallington 211 (1993) 41

Bally, T., L. Truttmann, S. Dai, J.T. Wang and F. Williams, The radical cation of 1,4-dihydropentalene and its photochemical formation from bicyclo[3.3.0]octa-2,6-diene-4,8-diyl cation 212 (1993) 141
Balucani, N., P. Casavecchia, D. Stranges and G.G. Volpi, The enthalpy of formation of the HSO radical 211 (1993) 469
Bañares, L., see F.J. Aoiz 218 (1994) 422
Bancewicz, T., Translational spectral moments for induction operators of non-multipolar form 213 (1993) 363
Bandow, S., see J.M. Holden 220 (1994) 186
Bao, Y., see M. Gong 217 (1994) 210
Bao, Y., see X. Song 217 (1994) 216
Baonza, V.G., M. Cáceres and J. Núñez, The spinodal as a reference curve for the high-pressure volumetric behavior of liquids 216 (1993) 579
Bar, I., see S. Koppe 214 (1993) 546
Baram, A., I. Last and M. Baer, Quantum-mechanical cross sections for the $D+H_2$ and $H+D_2$ reactive systems. Application of the negative imaginary potentials within the j_z approximation 212 (1993) 649
Baram, A., I. Last and M. Bear, Quantum-mechanical cross sections for the $D+H_2$ and $H+D_2$ reactive systems. Application of the negative imaginary potentials within the j_z approximation (Chem. Phys. Letters 212 (1993) 649). Erratum 215 (1993) 416
Baranyai, A., see I. Borzsák 216 (1993) 329
Barbedette, L., see P.M. Ajayan 215 (1993) 509
Barlow, M.J., see S. Clough 211 (1993) 637
Barnabas, M.V., see K.R. Cromack 218 (1994) 485
Barone, V., C. Adamo and N. Russo, Density functional approach to the structures and EPR parameters of open shell systems. The case of fluorovinyl radicals 212 (1993) 5
Barone, V. and P. Cristinziano, Theoretical investigation of the torsional potential of 2,2′-bipyrimidine 215 (1993) 40
Baros, F., see A.T. Reis e Sousa 213 (1993) 333
Barrans, Y., see M. Lequan 213 (1993) 71
Barrie, P.J., C.J. Groombridge, J. Mason and E.A. Moore, Nitrogen-15 nuclear magnetic shielding tensors in nitrite and nitrate ion. Experimental and theoretical determinations 219 (1994) 491
Barrois, R., see A. Lüchow 216 (1993) 359
Barrow, R.F., J. Chevaleyre, C. Effantin, M.A. Lebeault-Dorget, A.J. Ross, G. Wannous and J. Vergès, Electronic states of the Bi_2 molecule 214 (1993) 293
Bartelt, N.C., see B. Li 217 (1994) 595
Barthelat, J.C., see J. Rubio 217 (1994) 283
Bartlett, R.J., see L. Meissner 212 (1993) 177
Bartlett, R.J., see P.G. Szalay 214 (1993) 481
Bartlett, R.J., see S.A. Perera 216 (1993) 606
Barton, J.J., see B.L. Petersen 213 (1993) 412; 220 (1994) 46
Bartram, S., see S. Grimme 213 (1993) 32
Barzoukas, M., see M. Lequan 213 (1993) 71
Barzykin, A.V. and M. Tachiya, Generalized model for collisonal exchange of solubilized molecules in microdisperse systems 216 (1993) 575
Baskin, J.S., A. Saury and E. Carrasquillo M., Collisional approach to the spectroscopy of highly vibrationally excited HCN 214 (1993) 257

Bässler, H., see O. Dippel 216 (1993) 418
Baştuğ, T., D. Heinemann, W.-D. Sepp, D. Kolb and B. Fricke, All-electron Dirac–Fock–Slater SCF calculations of the Au_2 molecule 211 (1993) 119
Batchelor, S.N., K.A. McLauchlan and I.A. Shkrob, Spin-selective recombination in geminate radical pairs involving electronically excited radicals studied by MFE and CIDEP 214 (1993) 507
Battezzati, M., The diffusion equation for a mechanical system in the high-friction limit 216 (1993) 585
Bätz, P., see P. Lemoine 220 (1994) 177
Baugh, D.A., D.Y. Kim, V.A. Cho, L.C. Pipes, J.C. Petteway and C.D. Fuglesang, Production of a pure, single ro-vibrational quantum-state molecular beam 219 (1994) 207
Baughman, R.H. and D.S. Galvão, Tubulanes: carbon phases based on cross-linked fullerene tubules 211 (1993) 110
Baum, G. and J.R. Huber, Photodissociation of CF_2BrCl at 193 nm investigated by photofragment translational spectroscopy 213 (1993) 427
Bauschlicher Jr., C.W., see S.R. Langhoff 211 (1993) 305
Bauschlicher Jr., C.W., H. Partridge and S.R. Langhoff, Theoretical study of the NO b $^4\Sigma^-$ and O_2^+ b $^4\Sigma_g^-$ radiative lifetimes 211 (1993) 312
Bauschlicher Jr., C.W., see M. Sodupe 212 (1993) 624
Bauschlicher Jr., C.W. and M. Sodupe, A study of the ground and low-lying states of $MgCH_4^+$ 214 (1993) 489
Bauschlicher Jr., C.W. and H. Partridge, The vibrational frequencies of CH_2OH 215 (1993) 451
Bauschlicher Jr., C.W., S.R. Langhoff and H. Partridge, Theoretical study of the electronic states of MgC 216 (1993) 341
Bayer, E., W. Rossner, B.C. Grabmaier, R. Alcalá and G. Blasse, Time-resolved emission spectroscopy of Pr^{3+} in a fluoride glass 216 (1993) 228
Bear, M., see A. Baram 215 (1993) 416
Bearpark, M.J., M.A. Robb, F. Bernardi and M. Olivucci, Molecular mechanics valence bond methods for large active spaces. Application to conjugated polycyclic hydrocarbons 217 (1994) 513
Belinky, A., see A. Fernández 212 (1993) 201
Beljonne, D., see M. Fahlman 214 (1993) 327
Belyaev, J., see S. Fedrigo 211 (1993) 166
Benavides-Garcia, M. and K. Balasubramanian, Spectroscopic constants and potential energy curves of PbBr 211 (1993) 631
Benetis, N.P., A.S. Mahgoub, A. Lund and U. Nordh, Rotation of deuterated methylene groups in the diffusional regime. Isotope effect of anisotropic α-deuterons on ESR lineshapes of $^{\cdot}CD_2$–COO^- radical in irradiated ZnAC dihydrate single crystal 218 (1994) 551
Bénière, F.M., A. Boutin, M. Trache and A.H. Fuchs, Structural properties of $(SF_6)_{13}$ and $(SF_6)_{55}$ clusters by molecular dynamics simulation 215 (1993) 301
Ben-Itzhak, I., I. Gertner, O. Heber and B. Rosner, Formation and mean lifetime measurements of the long-lived doubly charged $HeNe^{2+}$ rare-gas dimer 212 (1993) 467
Bennema, P., see X.-Y. Liu 220 (1994) 53
Ben-Nun, M. and R.D. Levine, Stabilization of ion–molecule pairs by solvation 214 (1993) 175
Ben-Nun, M., T. Raz and R.D. Levine, Ballistic and dissociative collisions of a rare-gas atom with a halogen molecule 220 (1994) 291
Berezhkovskii, A.M. and V.Yu. Zitserman, Multi-dimensional Kramers theory of the reaction rate with highly anisotropic friction. Energy diffusion for the fast coordinate versus overdamped regime for the slow coordinate 212 (1993) 413

Berg, C., W. Wachter, T. Schindler, C. Kronseder, G. Niedner-Schatteburg, V.E. Bondybey and Z. Herman, Use of isotopic labeling in establishing reaction mechanisms: $CD_3^+ + C_2H_6$ 216 (1993) 465
Berkowitz, M.L., see L.S. Sremaniak 218 (1994) 377
Berman, A., H. Levanon, E. Vogel and N. Jux, Triplet spin alignment of "stretched porphycenes" 211 (1993) 549
Bernardi, F., see M.J. Bearpark 217 (1994) 513
Bernath, P.F., see L. Nemes 218 (1994) 295
Bernholc, J., see C.J. Brabec 219 (1994) 473
Bernier, P., see P.M. Ajayan 215 (1993) 509
Bertault, M., see J. Sworakowski 220 (1994) 197
Besenbacher, F., see M. Foss 215 (1993) 535
Bethune, D.S., see C.-H. Park 213 (1993) 196
Bezel, I.V., S.V. Chekalin, Yu.A. Matveets, A.G. Stepanov, A.P. Yartsev and V.S. Letokhov, Two-photon absorption of powerful femtosecond pulses in C_{60} film 218 (1994) 475
Bhat, S.G.T., see R.V. Jasra 211 (1993) 214
Bhattacharyya, K., see N. Sarkar 218 (1994) 492
Bhattacharyya, S.P., see P. Dutta 212 (1993) 677
Bi, X., see Y. Wang 217 (1994) 413
Bi, X.-X., see Y. Wang 211 (1993) 341
Bi, X.-X., see J.M. Holden 220 (1994) 186
Bierl, R., see S. Schneider 219 (1994) 433
Biermann, M., see M. Neeb 212 (1993) 205
Bieze, T.W.N., J.R.C. van der Maarel and J.C. Leyte, The intramolecular OH bond length of water in a concentrated poly(ethyleneoxide) solution. An NMR relaxation study 216 (1993) 56
Bigot, B., see S.A. Borshch 212 (1993) 398
Bill, H., see C. Pédrini 220 (1994) 433
Billing, G.D. and R.E. Kolesnick, Semi-classical calculations of rate constants for vibrational transitions in hydrogen 215 (1993) 571
Billing, G.D., see L. Goubert 219 (1994) 360
Bintz, K.L., D.L. Thompson, K.L. Kompa and R.D. Levine, The direct overtone pumping of polyatomic molecules 215 (1993) 455
Bird, D.M., L.J. Clarke, M.C. Payne and I. Stich, Dissociation of H_2 on Mg(0001) 212 (1993) 518
Bird, D.M., see J.A. White 213 (1993) 422
Bishop, D.M. and S.M. Cybulski, Calculation of electromagnetic properties of the noble gases 211 (1993) 255
Bisht, P.B., H. Petek and K. Yoshihara, Exciplex formation in van der Waals complexes of naphthalene–triethylamine in a supersonic jet 213 (1993) 75
Bist, H.D., see R.K. Singh 213 (1993) 210
Bittl, R., see A. Van der Est 212 (1993) 561
Bittl, R., Matrix elements of spin operators in exchange coupled tetrameric metal clusters 215 (1993) 279
Blain, M., see L. Koubi 217 (1994) 544
Blake, G.A., see P.A. Stockman 212 (1993) 298
Blasberg, T. and D. Suter, Nuclear spin relaxation of Pr^{3+} in $YAlO_3$. A temperature-dependent optical–rf double-resonance study 215 (1993) 668
Blasse, G., G.J. Dirksen, P. Zhiwu, G. Wehrum and R. Hoppe, Luminescence and energy migration in Ba_3NaNbO_6 and Ba_3NaTaO_6 215 (1993) 363

Blasse, G., see E. Bayer 216 (1993) 228
Blau, W.J., see P. Lemoine 220 (1994) 177
Blechta, V. and R. Freeman, Multi-site Hadamard NMR spectroscopy 215 (1993) 341
Blonski, S. and S.H. Garofalini, Molecular dynamics simulations of γ-alumina surface stabilization by deposited silicon ions 211 (1993) 575
Bludau, H., M. Gierer, H. Over and G. Ertl, A low-energy electron diffraction analysis of the $(\sqrt{3}\times\sqrt{3})$R30° structure of molecular nitrogen adsorbed on Ru(0001) 219 (1994) 452
Bludský, O., see R. Kobayashi 215 (1993) 576
Bo, C., see C. Sousa 215 (1993) 97
Bodenhausen, G., see S. Nicula 219 (1994) 291
Bodesheim, M., see R. Schmidt 213 (1993) 111
Bolender, J.P., D.H. Metcalf and F.S. Richardson, Chirality-dependent intermolecular interactions probed by time-resolved chiroptical luminescence measurements of enantiodifferential excited-state quenching kinetics 213 (1993) 131
Bollati, R.A. and J.C. Ferrero, Quasiclassical trajectory calculations of the transition probability function in the vibrational relaxation of HgBr($B\ ^2\Sigma$, $v=52$) by monoatomic gases 218 (1994) 159
Bonačić-Koutecký, V., P. Fantucci, C. Fuchs, C. Gatti, J. Pittner and S. Polezzo, Ab initio predictions of optically allowed transitions in Na_{20}. Nature of excitations and influence of geometry 213 (1993) 522
Bond, P., P.N. , J. Fletcher, P.A. Gorry and M.E. Pemble, Reactive scattering of Cl_2 on GaAs (100). Cl_2 and GaCl product distributions (Chem. Phys. Lett. 208 (1993) 269). Erratum 211 (1993) 649
Bondybey, V.E., see N. Caspary 212 (1993) 329
Bondybey, V.E., see M. Fárník 216 (1993) 458
Bondybey, V.E., see C. Berg 216 (1993) 465
Bondybey, V.E., see G. Schallmoser 219 (1994) 101
Bonneau, M., see S. Douin 216 (1993) 215
Bonnet, L., J.C. Rayez and P. Halvick, A geometric model for the regular dynamical behaviour of collinear three-atom reactions involving an intermediate well 216 (1993) 11
Bonosi, F., see G. Ricciardi 215 (1993) 541
Bonser, D., see L.A. Keeling 217 (1994) 136
Boo, D.W. and Y.T. Lee, Infrared spectra of CH_5^+ core in $CH_5^+(H_2)$ 211 (1993) 358
Boogaarts, M.G.H., see G. Meijer 217 (1994) 112
Booth, C., see C.-H. Park 213 (1993) 196
Booze, J.A., see D.E. Govoni 216 (1993) 525
Boraas, K., see Z. Lin 217 (1994) 239
Borg, R.A.J., E.R. Waclawik, Mudjijono and W.D. Lawrance, A strong collision partner dependence for vibrational energy transfer in benzene and benzene-d_6. He versus D_2 218 (1994) 320
Borrás-Almenar, J.J., E. Coronado, H.M. Kishinevsky and B.S. Tsukerblat, Semiclassical approximation in the magnetic problem of exchange-coupled mixed valence clusters 217 (1994) 525
Borrmann, A., see L.M. Finney 214 (1993) 159
Borrmann, A., see Z. Li 214 (1993) 362
Borshch, S.A. and B. Bigot, Magnetic properties of the mixed-valence heteropoly blues with a Keggin structure 212 (1993) 398
Borzsák, I. and A. Baranyai, The overlap volume in hard spheres under shear 216 (1993) 329
Botella, V., O. Castaño, P. Fernández-Serra and Y.G. Smeyers, Multiple solutions and spatial symmetry properties of singlet and triplet states in the half-projected Hartree–Fock method 219 (1994) 497

Botschwina, P., M. Oswald, J. Flügge, Ä. Heyl and R. Oswald, Ab initio spectroscopic constants and the equilibrium geometry of HCCF (Chem. Phys. Letters 209 (1993) 117). Erratum 215 (1993) 681
Boulon, G., see J.A. Mares 217 (1994) 105
Boustani, I., see H.-P. Liebermann 214 (1993) 381
Boutin, A., see F.M. Bénière 215 (1993) 301
Boutin, A., B. Rousseau and A.H. Fuchs, The temperature–size phase diagram of large SF_6 clusters by computer simulation 218 (1994) 122
Boutin, A., R.J.-M. Pellenq and D. Nicholson, Molecular simulation of the stepped adsorption isotherm of methane in $AlPO_4$-5 219 (1994) 484
Bouttet, D., see C. Pédrini 220 (1994) 433
Bowers, M.T., see G. von Helden 212 (1993) 241, 247
Bowman, J.M., A test of an adiabatic treatment of rotation for vibration/rotation energies of polyatomic molecules 217 (1994) 36
Boyd, R.J., see L.A. Eriksson 211 (1993) 88
Boyd, R.J., see J. Kong 217 (1994) 24
Brabec, C.J., A. Maiti and J. Bernholc, Structural defects and the shape of large fullerenes 219 (1994) 473
Bradley, A., see J.S. Francisco 214 (1993) 77
Bradshaw, A.M., see M. Neeb 212 (1993) 205
Bradshaw, A.M., see B. Rausenberger 215 (1993) 109
Bradshaw, A.M., see M. Ondřejček 215 (1993) 528
Braga, M. and S. Larsson, Correlation and relaxation effects in the electronic coupling between acetylenic π and π* electrons through saturated and aromatic spacers 213 (1993) 217
Bramble, S.K., see J. Baker 213 (1993) 297
Brand, H.R., see M. Diewald 216 (1993) 566
Brandl, V., see O. Dippel 216 (1993) 418
Braun, C.L., see S.N. Smirnov 217 (1994) 167
Braune, M. and H. Engel, Compound rotation of spiral waves in active media with periodically modulated excitability 211 (1993) 534
Bravic, G., see M. Lequan 213 (1993) 71
Bréchignac, P., see S. Douin 216 (1993) 215
Brédas, J.L., see M. Fahlman 214 (1993) 327
Brédas, J.L. and A.J. Heeger, Influence of donor and acceptor substituents on the electronic characteristics of poly(paraphenylene vinylene) and poly(paraphenylene) 217 (1994) 507
Breest, A., see S. Grimme 213 (1993) 32
Breheret, E., see F. Lahmani 220 (1994) 235
Breidohr, R., O. Shestakov and E.H. Fink, The a $^3\Sigma_u^+$ $(a_1 1_u) \rightarrow X\ ^1\Sigma_g^+ (X0_g^+)$ transition of Sb_2 218 (1994) 13
Brendsdal, E., see I. Gutman 219 (1994) 355
Brenier, A., see J.A. Mares 217 (1994) 105
Brenner, L.J., J. Senekowitsch and R.E. Wyatt, Coupled cluster calculation of the in-plane harmonic force field of benzene 215 (1993) 63
Breton, J. and E. Nabedryk, $S_0 \rightarrow T_1$ infrared difference spectrum of the triplet state of the primary electron donor in *Rb. sphaeroides* photosynthetic bacterial reaction centers 213 (1993) 571
Bridges, F., see C.-H. Park 213 (1993) 196
Brier, P.N., see P. Bond 211 (1993) 649
Brillante, A., M. Cau, R.G. Della Valle and E. Venuti, The effect of pressure on the photodimerization of 7-methoxycoumarin crystal 218 (1994) 568

Brink, C., see L.H. Andersen 217 (1994) 204
Brion, J., A. Chakir, D. Daumont, J. Malicet and C. Parisse, High-resolution laboratory absorption cross section of O_3. Temperature effect 213 (1993) 610
Brocklehurst, B., Radio-luminescence of alkane solutions. Comparison of experiment and simulation over a wide energy range 211 (1993) 31
Bronnikov, D.K., see A.E. Wiskerke 216 (1993) 93
Broström, L., see G. Sundström 218 (1994) 17
Brouard, M., see M. Baba 220 (1994) 411
Brouwer, A.M., see S.I. van Dijk 214 (1993) 502
Brown, R.J.C., see P.W. Fowler 216 (1993) 200
Broyer, M., see K. Kobe 213 (1993) 554
Broyer, M., see M. Pellarin 217 (1994) 349
Brugmans, M.J.P., A.W. Kleyn, A. Lagendijk, W.P.J.H. Jacobs and R.A. van Santen, Hydrogen bonding in acidic zeolites observed by time-resolved vibrational spectroscopy 217 (1994) 117
Brühwiler, P.A., S. Andersson, M. Dippel, N. Mårtensson, P.A. Demirev and B.U.R. Sundqvist, Hydrogenation of solid C_{60} by atomic hydrogen 214 (1993) 45
Brunvoll, J., see I. Gutman 219 (1994) 355
Brusa, R.S., see G. Karwasz 211 (1993) 529
Buchachenko, A.A., A.Yu. Baisogolov and N.F. Stepanov, The vibrational predissociation lifetime of the He...N_2^+ (X, $v=1$) complex 220 (1994) 93
Büchel, M., see Z. Sekkat 220 (1994) 497
Buchen, Th. and P. Gütlich, Thermal and light-induced spin crossover in iron(II) complexes with monodentate tetrazole ligands carrying long alkyl chains in the 1-position 220 (1994) 262
Buckingham, A.D. and R.M. Olegário, Hyperfine coupling in alkaline earth monofluorides. Limitations of the ionic model 212 (1993) 253
Buenker, R.J., see Y. Li 212 (1993) 185
Buenker, R.J., see H.-P. Liebermann 214 (1993) 381
Bulanin, M.O., Spectral interpretation of the refractivity and dielectric virial coefficients of atomic gases 217 (1994) 466
Bungay, A.R., S.V. Popov, Yu.P. Svirko and N.I. Zheludev, Time-non-invariant linear birefringence and dichroism due to spin–orbit interaction 217 (1994) 249
Buntine, M.A., D.J. Lavrich, C.E. Dessent, M.G. Scarton and M.A. Johnson, Photoinitiation of the $O^- + H_2O \rightarrow OH^- + OH$ ion–molecule reaction within the $O_2^- \cdot H_2O$ binary complex 216 (1993) 471
Burba, M.E., see S.K. Lim 216 (1993) 405
Burg, B., see R. Koch 220 (1994) 172
Burgard, C., see S.A. Dikanov 212 (1993) 493
Burgers, P.C., see G.A. McGibbon 218 (1994) 499
Burke, L.A., see P.N. Krishnan 217 (1994) 311
Burn, P.L., see I.D.W. Samuel 213 (1993) 472
Burrows, P.E., see E.I. Haskal 219 (1994) 325
Burshtein, Z., see R. Gvishi 212 (1993) 463; 213 (1993) 338
Burt, J.A. and G.A. Crosby, Barriers to energy migration in mixed-ligand zinc(II) complexes 220 (1994) 493
Burton, N.A., see R.J. Hall 220 (1994) 129
Butler, D.A., B.E. Hayden and J.D. Jones, Precursor dynamics in dissociative hydrogen adsorption on W(100) 217 (1994) 423
Buttet, J., see S. Fedrigo 211 (1993) 166
Byrne, H.J., see L. Akselrod 212 (1993) 384; 215 (1993) 131

Caballol, R., see À. Povill 218 (1994) 283
Cáceres, M., see V.G. Baonza 216 (1993) 579
Cahill, P.A., see C.C. Henderson 213 (1993) 383
Cai, Z.-L., X.-G. Zhang and X.-Y. Wang, Ab initio study of four low-lying electronic states of the CCS molecule 213 (1993) 168
Cai, Z.-L. and J.-L. Bai, Ab initio study of the electronic spectrum of the SF_2 radical 220 (1994) 109
Caldiño G., U., M. Voda, F. Jaque, J. García Solé and A.A. Kaminskii, Nd^{3+} multisites in the disordered $Ca_3Ga_2Ge_3O_{12}$ laser crystal 213 (1993) 84
Caldwell, C.D., see S.J. Schaphorst 213 (1993) 315
Calvo Hernández, A., see J.M.M. Roco 216 (1993) 593
Campargue, A., see A. Charvát 214 (1993) 495
Canet, D., J.B. Robert and P. Tekely, ^{13}C NMR relaxation time of fullerene as a function of magnetic field 212 (1993) 483
Cao, D., see Y. Chen 211 (1993) 449
Capitelli, M., see G. Colonna 213 (1993) 5
Carlson, M., see G. Sundström 218 (1994) 17
Carnell, M. and S.D. Peyerimhoff, Assignment of the vacuum-ultraviolet spectrum of ethylene sulphide 212 (1993) 654
Carrasquillo M., E., see J.S. Baskin 214 (1993) 257
Carrasquillo M., E., see R. Huang 216 (1993) 108, 115
Carrington, A., C.A. Leach, A.J. Marr, C.H. Pyne, A.M. Shaw, M.R. Viant and Y.D. West, Near-dissociation microwave spectra of rare-gas diatomic ions 212 (1993) 473
Carruthers, J.R., see J.D. Gale 216 (1993) 155
Carter, E.A., see B. Hartke 216 (1993) 324
Cartier, S.F., B.D. May, B.J. Toleno, J. Purnell, S. Wei and A.W. Castleman Jr., The production of metallocarbohedrenes by the direct laser vaporization of the carbides of titanium and zirconium 220 (1994) 23
Cartland, H.E., see B.M. Rice 211 (1993) 283
Casavecchia, P., see N. Balucani 211 (1993) 469
Caselli, M., F. Momicchioli and G. Ponterini, Modelling of the cis–trans partitioning in the photoisomerizations of cyanines and stilbene derivatives 216 (1993) 41
Caspar, J.V. and Y. Wang, Excited state electron transfer of fullerenes. Singlet states versus triplet states 218 (1994) 221
Caspary, N., B.E. Wurfel, A. Thoma, G. Schallmoser and V.E. Bondybey, Infrared identification of the FCS radical in an argon matrix 212 (1993) 329
Cassidei, L., see G. Petrella 212 (1993) 512
Castanheira, E.M.S., see A.T. Reis e Sousa 213 (1993) 333
Castaño, O., see V. Botella 219 (1994) 497
Casties, A., see J. Mai 211 (1993) 197
Castillejo, M., J.M. Figuera, H.A. Zeaiter and M. Oujja, Rate constants for removal by noble gases of selected rotational levels of methylene $^1B_1(0, 14, 0)$ 214 (1993) 227
Castleman Jr., A.W., see S.F. Cartier 220 (1994) 23
Castleman Jr., A.W., see Z. Shi 220 (1994) 274
Catlow, C.R.A., see J.D. Gale 216 (1993) 155
Cau, M., see A. Brillante 218 (1994) 568
Caubet, P. and G. Dorthe, Origin of C_2 high-pressure bands observed in the products of a microwave discharge through CO 218 (1994) 529

Causà, M. and A. Zupan, Density functional LCAO calculation of periodic systems. A posteriori correction of the Hartree–Fock energy of covalent and ionic crystals 220 (1994) 145
Cazzini, K., see P. Lemoine 220 (1994) 177
Cazzoli, G., see C. Degli Esposti 214 (1993) 531
Cederbaum, L.S., see M.K. Scheller 216 (1993) 141
Cemic, F., see K.W. Kolasinski 219 (1994) 113
Céolin, R., see B. Keita 215 (1993) 125
Ceulemans, A. and G. Mys, The vector particle of tensor surface harmonic theory 219 (1994) 274
Cháb, V., see M. Ondřejček 215 (1993) 528
Chabach, D., see T.-H. Tran-Thi 213 (1993) 139
Chabalowski, C.F., see B.M. Rice 211 (1993) 283
Chakir, A., see J. Brion 213 (1993) 610
Chakrabarti, A., S. Yashonath and C.N.R. Rao, Orientational glassy phases of C_{60} and neopentane. A Monte Carlo study 215 (1993) 591
Chakravorty, S.J., see E.R. Davidson 217 (1994) 48
Chambaud, G., see A. Spielfiedel 216 (1993) 162
Chambers, C.C. and D.L. Thompson, Enhancement of vibrational mode mixing due to isomerization barrier crossings 218 (1994) 166
Champagne, B. and Y. Öhrn, Ab initio longitudinal polarizabilities of conjugated stereoregular polymers with a carbon backbone 217 (1994) 551
Chan, I.Y., C.M. Wong and D. Stehlik, Pressure dependence of the low-temperature tunneling rate for the hydrogen transfer in acridine-doped fluorene crystals 219 (1994) 187
Chan, M.-C., see B. Fain 216 (1993) 551
Chandler, C., see W. Zhu 217 (1994) 73
Chandrasekhar, J., see S.P. Ananthavel 217 (1994) 101
Chang, C.P., see P.-T. Chou 216 (1993) 300; 220 (1994) 229
Chang, H., see C.-C. Chen 217 (1994) 486
Chang, R.K., see J.L. Cheung 213 (1993) 309
Chang, S.-H., see R.C. Haddon 218 (1994) 100
Chang, T.-C., H.-W. Li, T.-C. Hsieh and S.-H. Chou, Picosecond time-resolved CSRS study of vibrational dephasing of bulk modes perturbed by electronic state of dilute impurities 213 (1993) 564
Chang, T.C., see B. Fain 216 (1993) 551
Chao, M., see P.-T. Chou 220 (1994) 229
Charra, F., see J.-M. Nunzi 215 (1993) 114; 219 (1994) 349
Charvát, A., A.A. Kachanov, A. Campargue, D. Permogorov and F. Stoeckel, High sensitivity intracavity absorption spectroscopy of CHD_3 in the near infrared with a titanium:sapphire laser 214 (1993) 495
Chasseau, D., see M. Lequan 213 (1993) 71
Châtelain, A., see W.S. Bacsa 211 (1993) 346
Chattaraj, P.K., S. Nath and A.B. Sannigrahi, Ab initio SCF study of maximum hardness and maximum molecular valency principles 212 (1993) 223
Chattaraj, P.K. and S. Nath, Hardness dynamics in a chemical reaction 217 (1994) 342
Chaudhuri, J., see R. Debnath 217 (1994) 357
Chavy, C., C. Joachim and A. Altibelli, Interpretation of STM images: C_{60} on the gold(110) surface 214 (1993) 569
Chavy, C., C. Joachim and A. Altibelli, Interpretation of STM images: C_{60} on the gold(110) surface (Chem. Phys. Letters 214 (1993) 569). Erratum 219 (1994) 502

Chekalin, S.V., see I.V. Bezel 218 (1994) 475
Chemerisov, S.D., O.Ya. Grinberg, D.S. Tipikin, Ya.S. Lebedev, H. Kurreck and K. Möbius, Mechanically induced radical pair formation in porphyrin–quinone and related donor–acceptor mixtures. Unusual stability and zero-field splittings 218 (1994) 353
Chemseddine, A., Fibrous and oriented quantum dots. Synthesis and characterization 216 (1993) 265
Chen, C., see Y. Chen 211 (1993) 449
Chen, C.-C., H. Chang and C.-S. Hsue, A highly accurate calculation for the electronic states of H_2^+ in B-spline basis 217 (1994) 486
Chen, C.H., see R.B. Jones 212 (1993) 451
Chen, J. and P.J. Dagdigian, Spectrally resolved fluorescence in the HNF (DNF) $\tilde{A}\ ^2A'$–$\tilde{X}\ ^2A''$ band system 213 (1993) 586
Chen, K. and C. Pei, Time-resolved intensity patterns of photofragments by laser sheet illumination and two-dimensional imaging techniques 217 (1994) 471
Chen, L., see L.A. Keeling 217 (1994) 136
Chen, X., see H. Wang 216 (1993) 537
Chen, Y., C. Chen, X. Ma, S. Li, Y. Chu and D. Cao, Energy transfer reaction for CS with metastable CO(a) 211 (1993) 449
Cheng, P.Y., see P. DeRose 220 (1994) 207
Cheng, W.-D., J.-S. Huuang and Q.-E. Zhang, Electronic structure of the ground state and calculated spectrum of low-lying excited states of $Mo_3X_4(aq)_9^{4+}$ (X=O, S) cluster ions 216 (1993) 353
Chergui, M., R. Reininger, E. Morikawa and A. Tramer, Control by density effects of the Rydberg–valence configuration mixing in matrix isolated NO 216 (1993) 34
Chergui, M. and N. Schwentner, Experimental evidence to Rydbergization of antibonding molecular orbitals 219 (1994) 237
Chermette, H., see F. Rogemond 219 (1994) 228
Chernia, Z. and D. Gill, Reversible self-assembly of fluorescent dimers of anthracene derivative adsorbed on laponite 212 (1993) 57
Chernozatonskii, L.A., see E.G. Gal'pern 214 (1993) 345
Chernozatonskii, L.A., see A.A. Kharlamov 219 (1994) 457
Cheskis, S., see A.A. Iogansen 212 (1993) 604
Cheung, J.L., A.S. Kwok, K.A. Juvan, D.H. Leach and R.K. Chang, Stimulated low-frequency emission from anisotropic molecules in microdroplets 213 (1993) 309
Chevaleyre, J., see R.F. Barrow 214 (1993) 293
Ching, K.C., see M. Lequan 213 (1993) 71
Chistykov, A.L., see E.G. Gal'pern 214 (1993) 345
Chitta, V., see S. Astilean 219 (1994) 95
Chiu, C.L., see Y.R. Lee 216 (1993) 209
Chiu, S.-W., see Z.-X. Ma 213 (1993) 250
Chmelka, B.F., see R.G. Larsen 214 (1993) 220
Cho, S.J., see K.S. Kim 216 (1993) 309
Cho, V.A., see D.A. Baugh 219 (1994) 207
Chong, D.P., Local density calculations of static dielectric properties of $CH_{4-n}Cl_n$, $n=0$–4 217 (1994) 539
Chong, D.P., Local density studies of diatomic AB molecules, A, B=C, N, O, F, Si, P, S, and Cl 220 (1994) 102
Chorkendorff, I., see J. Hall 216 (1993) 413
Chou, P.-T., W.C. Cooper, J.H. Clements, S.L. Studer and C.P. Chang, A comparative study. The photophysics of 2-phenylbenzoxazoles and 2-phenylbenzothiazoles 216 (1993) 300

Chou, P.-T., M. Chao, J.H. Clements, M.L. Martinez and C.-P. Chang, Excited-state intramolecular proton transfer for N-substituted-3-hydroxypyridinones 220 (1994) 229
Chou, S.-H., see T.-C. Chang 213 (1993) 564
Choudary, N.V., see R.V. Jasra 211 (1993) 214
Chowdhury, P.K., see Awadhesh Kumar 212 (1993) 103
Chowdhury, P.K., K.V.S. Rama Rao and J.P. Mittal, Infrared multiphoton dissociation of acrolein. Time-resolved observation of CO ($v=1$) IR emission at 4.7 μm 218 (1994) 60
Christensen, O.B. and J.K. Nørskov, Modeling the potassium promotion of CO bonding to Ni(100) 214 (1993) 443
Christmann, K., see R. Koch 220 (1994) 172
Chronister, E.L., see R.A. Crowell 216 (1993) 293
Chu, B., see Q. Ying 219 (1994) 214
Chu, K., G.U. Nienhaus and R. Philipp, Structural heterogeneity in proteins at cryogenic temperatures. Cooling rate dependence 216 (1993) 275
Chu, S.-I, see Y. Huang 211 (1993) 601
Chu, Y., see Y. Chen 211 (1993) 449
Chupka, W.A., see Y. Wang 214 (1993) 290
Chvoj, Z., see M. Ondřejček 215 (1993) 528
Ciesielski, W., see N.D. Kushch 215 (1993) 137
Cimiraglia, R. and H.-J. Hofmann, Rotation and inversion states in thermal E/Z isomerization of aromatic azo compounds 217 (1994) 430
Cioslowski, J., Heats of formation of higher fullerenes from ab initio Hartree–Fock and correlation energy functional calculations 216 (1993) 389
Cioslowski, J. and A. Nanayakkara, A new robust algorithm for fully automated determination of attractor interaction lines in molecules 219 (1994) 151
Clarke, L.J., see D.M. Bird 212 (1993) 518
Clarke, L.J., see I. Štich 212 (1993) 617
Clary, D.C., see S.K. Pogrebnya 219 (1994) 366
Clementi, E., see G. Corongiu 214 (1993) 367
Clements, J.H., see P.-T. Chou 216 (1993) 300; 220 (1994) 229
Cline, J.I., see J.L. Tomer 216 (1993) 286
Clough, S., A.J. Horsewill, A.M. Alsanoosi, M.J. Barlow and M.R. Johnson, The spectrum of rotating wavepackets of hindered methyl groups 211 (1993) 637
Coat, Y.L., see R. Azria 220 (1994) 417
Cockett, M.C.R., J.G. Goode, K.P. Lawley and R.J. Donovan, The spectroscopy of Rydberg excited iodine–argon van der Waals complexes 214 (1993) 27
Codling, K., see D.M. Smith 216 (1993) 493
Cohen, M. and T. Feldmann, The systematic derivation of realizations of generators of Lie algebras 218 (1994) 147
Cohen de Lara, E., see L. Koubi 217 (1994) 544
Colliex, C., see P.M. Ajayan 215 (1993) 509
Collings, B.A., see K. Athanassenas 213 (1993) 105
Collins, M.A., see F. Zhang 214 (1993) 459
Collins, S.J., see P.J. O'Malley 217 (1994) 293
Colonna, F. and E.M. Evleth, Conformationally invariant modeling of atomic charges 212 (1993) 665
Colonna, G., C. Gorse, M. Capitelli, R. Winkler and J. Wilhelm, The influence of electron–electron collisions on electron energy distribution functions in N_2 post discharge 213 (1993) 5

Columbia, M.R. and P.A. Thiel, The stabilization of formate on Pt(111) by coadsorbed atomic oxygen 220 (1994) 167
Colwell, S.M. and N.C. Handy, The determination of magnetisabilities using density functional theory 217 (1994) 271
Comelli, G., see D. Arvanitis 211 (1993) 53
Comelli, G., see C. Comicioli 214 (1993) 438
Comicioli, C., V.R. Dhanak, G. Comelli, C. Astaldi, K.C. Prince, R. Rosei, A. Atrei and E. Zanazzi, Structure of Rh{110}(1×2) and Rh{110}(2×2)p2mg-O surfaces 214 (1993) 438
Cong, P., H.P. Deuel and J.D. Simon, Using optical coherence to measure the ultrafast electronic dephasing of large molecules in room-temperature liquids 212 (1993) 367
Conrad, H., see M. Ondřejček 215 (1993) 528
Conwell, E.M., see Yu.N. Gartstein 217 (1994) 41
Coolidge, M., see R. Pandey 220 (1994) 337
Coombe, R.D., see S.M. Singleton 215 (1993) 237
Cooper, A.I. and M. Poliakoff, High-pressure reactions in polyethylene films, a new development in matrix isolation. The photochemical reaction of $Fe(CO)_5$ with N_2 and the thermal reaction of $Fe(CO)_4(N_2)$ with H_2 212 (1993) 611
Cooper, W.C., see P.-T. Chou 216 (1993) 300
Corchado, J.C., see J. Espinosa-Garcia 218 (1994) 128
Corn , R.M., see D.A. Higgins 213 (1993) 485
Coronado, E., see J.J. Borrás-Almenar 217 (1994) 525
Corongiu, G. and E. Clementi, Liquid water: density of states spectra of solvated water molecules with specific coordination 214 (1993) 367
Corval, A., see S. Astilean 219 (1994) 95
Cory, D.G., F.H. Laukien and W.E. Maas, NMR spectroscopy with radial pulses. p- and n-type selection COSY 212 (1993) 487
Cotts, R.M., see S. Miyajima 212 (1993) 277
Coussan, S., N. Bakkas, A. Loutellier, J.P. Perchard and S. Racine, Infrared photoisomerization of the methanol cyclic trimer trapped in a nitrogen matrix 217 (1994) 123
Couto, M.S., see X.-Y. Liu 220 (1994) 53
Coy, S., see G.M. Schmid 219 (1994) 331
Cramer, C.J., F.J. Dulles, J.W. Storer and S.E. Worthington, Full valence complete active space SCF, multireference CI, and density functional calculations of $^1A_1$–$^3B_1$ singlet–triplet gaps for the valence-isoelectronic series BH_2^-, CH_2, NH_2^+, AlH_2^-, SiH_2, PH_2^+, GaH_2^-, GeH_2, and AsH_2^+ 218 (1994) 387
Cremer, D., see L. Olsson 215 (1993) 433
Cremer, D., see E. Kraka 216 (1993) 333; 219 (1994) 160
Crespo, R., see M.C. Piqueras 213 (1993) 509
Crim, F.F., see D.E. Govoni 216 (1993) 525
Cristinziano, P., see V. Barone 215 (1993) 40
Croci, M., H.-J. Müschenborn, F. Güttler, A. Renn and U.P. Wild, Single molecule spectroscopy: pressure effect on pentacene in *p*-terphenyl 212 (1993) 71
Cromack, K.R., D.W. Werst, M.V. Barnabas and A.D. Trifunac, Low-temperature study of radical cations of quadricyclane and norbornadiene in Na-ZSM-5 zeolites 218 (1994) 485
Crosby, G.A., see J.A. Burt 220 (1994) 493
Crowell, R.A. and E.L. Chronister, A photon echo study of pentacene in naphthalene at high pressure 216 (1993) 293

Crystall, B., see I.D.W. Samuel 213 (1993) 472
Culver, J.P., M. Li, L.G. Jahn, R.M. Hochstrasser and A.G. Yodh, Vibrational response of surface adsorbates to femtosecond substrate heating 214 (1993) 431
Curtiss, L.A., K. Raghavachari and J.A. Pople, The accurate determination of enthalpies of formation 214 (1993) 183
Cvejanovic, S., see R. Abouaf 213 (1993) 503
Cybulski, S.M., see D.M. Bishop 211 (1993) 255
Cyr, D.R., see D.J. Leahy 216 (1993) 503
Cyvin, B.N., see I. Gutman 219 (1994) 355
Cyvin, S.J., see I. Gutman 219 (1994) 355
Czajkowski, A., see W. Kedzierski 218 (1994) 314
Czuchaj, E., F. Rebentrost, H. Stoll and H. Preuss, Calculation of the interaction energies for the ZnHg and ZnCd system 212 (1993) 534
Czuchaj, E., F. Rebentrost, H. Stoll and H. Preuss, Adiabatic potential curves for the KZn and KCd excimers 218 (1994) 454

Dadali, A.A., see J.M. Lang 214 (1993) 310
Dagdigian, P.J., see J. Chen 213 (1993) 586
Dai, H.L., see P. DeRose 220 (1994) 207
Dai, S., see T. Bally 212 (1993) 141
Dale, M.J., see A.C. Jones 219 (1994) 174
Dalgaard, E., see H. Koch 212 (1993) 193
Dang, L.X., Solvation of ammonium ion. A molecular dynamics simulation with nonadditive potentials 213 (1993) 541
D'Angelo, M., G. Onori and A. Santucci, Study of aggregation of *n*-butoxyethanol in water by compressibility and surface tension measurements 220 (1994) 59
Danieli, R., see O. Dippel 216 (1993) 418
Danieli, R., see F. Kajzar 217 (1994) 418
Dantus, M., see M.H.M. Janssen 214 (1993) 281
Dao, L., see T.-H. Tran-Thi 213 (1993) 139
Darmanyan, A.P., Mechanism of singlet oxygen interaction with solvent removing prohibition of the radiative $^1\Delta_g \rightarrow {}^3\Sigma_g^-$ transition in oxygen 215 (1993) 477
Das, A.K., see T.K. Ghosh 218 (1994) 433
Das, G.P., A.T. Yeates and D. Dudis, Vibronic contribution to static molecular hyperpolarizabilities 212 (1993) 671
Das, K., see N. Sarkar 218 (1994) 492
Dasannacharya, B.A., see P.S. Goyal 211 (1993) 559
Daschbach, J.L., see P.R. Fischer 218 (1994) 200
Das Chowdhury, K., see J.M. Holden 220 (1994) 186
Daumont, D., see J. Brion 213 (1993) 610
Davidson, E.R. and S.J. Chakravorty, A possible definition of basis set superposition error 217 (1994) 48
Davidsson, J., see L. Ming 211 (1993) 189
Davies, P.B., Y. Liu and Z. Liu, Far infrared LMR spectra of monobromomethyl radicals 214 (1993) 305
Davis, H.F., P.I. Ionov, S.I. Ionov and C. Wittig, Picosecond resolution measurements of NO_3 unimolecular decomposition. The $NO+O_2$ channel 215 (1993) 214
De Andrés, J., see A. Aguilar 220 (1994) 267
Debnath, R. and J. Chaudhuri, Coordination structure and the bonding properties of UV-laser-induced photo-generated Cu(II) in a monovalent copper containing silica glass 217 (1994) 357
De Boer, J.L., S. van Smaalen, V. Petricek, M. Dusek, M.A. Verheijen and G. Meijer, Hexagonal close-packed C_{60} 219 (1994) 469
De Caro, C., see H. van der Laan 212 (1993) 569
De Cian, A., see T.-H. Tran-Thi 213 (1993) 139
DeDios, A.C., see J.D. Augspurger 213 (1993) 211
Degli Esposti, C., F. Tamassia, G. Cazzoli and P. De Natale, High-resolution Fourier transform spectroscopy of the ν_1 fundamental band of nitrosyl bromide 214 (1993) 531
De Heer, W.A., see W.S. Bacsa 211 (1993) 346
Dehmer, J.L., see E.F. McCormack 211 (1993) 147
Dehmer, P.M., see E.F. McCormack 211 (1993) 147
Dekkers, H.P.J.M., see S.C.J. Meskers 216 (1993) 241
Delcourt, M.O., see S. Remita 218 (1994) 115
Della Valle, R.G., see A. Brillante 218 (1994) 568
Dement'ev, A.I., see V.I. Alexandrov 218 (1994) 206
Demirev, P.A., see P.A. Brühwiler 214 (1993) 45

De Natale, P., see C. Degli Esposti 214 (1993) 531
Deng, C., see S. Feng 214 (1993) 97
Denton, A.R., C.G. Gray and D.E. Sullivan, Orientational ordering of surfactant monolayers adsorbed at the air–water interface. Structural model and fit to neutron reflectivity data 219 (1994) 310
Depaemelaere, S., L. Viaene, M. Van der Auweraer, F.C. De Schryver, R.M. Hermant and J.W. Verhoeven, Non-radiative decay processes of the intramolecular charge transfer state in a rigid bichromophoric system 215 (1993) 649
Depero, L.E. and F. Parmigiani, A study of the electronic structure of decagonal $Al_{70}Ni_{15}Co_{15}$ quasi-crystal 214 (1993) 208
De Proft, F. and P. Geerlings, The effect of electron correlation on the shell structure of atoms 220 (1994) 405
DeRose, P., H.L. Dai and P.Y. Cheng, Degenerate four-wave mixing spectroscopy of the $(glyoxal)_2$ van der Waals complex 220 (1994) 207
De Santis, A., A. Gregori and D. Rocca, The range of the local order in a model of diatomic liquid 213 (1993) 239
De Schryver, F.C., see S. Depaemelaere 215 (1993) 649
De Silvestri, S., see M. Nisoli 220 (1994) 64
Desoppere, E., see L. Goubert 219 (1994) 360
Dessent, C.E., see M.A. Buntine 216 (1993) 471
Deuel, H.P., see P. Cong 212 (1993) 367
Deumens, E., see R. Longo 220 (1994) 305
De Vita, A., see I. Štich 212 (1993) 617
De Vries, M.S., see C.-H. Park 213 (1993) 196
Dhanak, V.R., see C. Comicioli 214 (1993) 438
Dibble, T.S. and J.S. Francisco, An ab initio study of the reaction of atomic fluorine and chlorine with trifluoroacetaldehyde 215 (1993) 409
Dibble, T.S. and J.S. Francisco, FNO_2: improving calculated structures at the second-order Møller–Plesset level of theory 215 (1993) 423
Di Bella, S., G. Lanza and I.L. Fragalà, Equilibrium geometries and harmonic vibrational frequencies of lanthanum trihalides LaX_3 (X = F, Cl). A relativistic effective core potential ab initio MO study 214 (1993) 598
DiCarlo, J., see C.-H. Park 213 (1993) 196
Dietz, K., C. Schmidt, M. Warken and B.A. Heß, Explicit construction of a convergent MBPT series for the $^1\Delta$ state of C_2 and the H_2 ground state at large bond distance 220 (1994) 397
Diewald, M. and H.R. Brand, Chemically driven convection. A simple model 216 (1993) 566
Dikanov, S.A., C. Burgard and J. Hüttermann, Determination of the hyperfine coupling with the remote nitrogen in the VO^{2+}–$(imidazole)_4$ complex by ESEEM spectroscopy 212 (1993) 493
Ding, G., W. Yang, W. Sun, D. Xu, G. He and N. Lou, The product polarization of chemiluminescent reactions of orbital aligned $Ca(^1P_1)$ with CH_3I and C_2H_5I 220 (1994) 1
Ding, L.N., M.A. Young, P.D. Kleiber and W.C. Stwalley, Photofragmentation spectroscopy of $Mg_2CO_2^+$ 212 (1993) 499
Diniz, R.E.O., see S.J.L. Ribeiro 220 (1994) 214
Dippel, M., see P.A. Brühwiler 214 (1993) 45
Dippel, O., V. Brandl, H. Bässler, R. Danieli, R. Zamboni and C. Taliani, Energy-dependent branching between fluorescence and singlet exciton dissociation in sexithienyl thin films 216 (1993) 418

Dirksen, G.J., see G. Blasse 215 (1993) 363
Dityat'ev, A.A., see A.A. Kharlamov 219 (1994) 457
Diz, A., see R. Longo 220 (1994) 305
Dolejšek, Z., see M. Fárník 216 (1993) 458
Doleman, B.J., see S.M. Mattar 216 (1993) 369
Dolg, M., see P. Schwerdtfeger 218 (1994) 362
Dolg, M., see D. Andrae 220 (1994) 341
Doll, J.D., see A.B. Finnila 219 (1994) 343
Dolson, D.A., A. Liu and K.M. Schreier, Infrared fluorescence observations of electronic to vibrational energy transfer from $Br^*(4\ ^2P_{1/2})$ to SO_2 212 (1993) 118
Dolson, D.A. and D.S. West, Infrared fluorescence observations of electronic to vibrational energy transfer from $Cl^*\ [3p^5(^2P_{1/2})]$ to SO_2 216 (1993) 258
Domcke, W., see A.L. Sobolewski 211 (1993) 82
Domcke, W. and C. Woywod, Direct construction of diabatic states in the CASSCF approach. Application to the conical intersection of the $^1A_2$ and $^1B_1$ excited states of ozone 216 (1993) 362
Domke, M., see G. Remmers 214 (1993) 241
Dong, Z.-H., see P. Zhou 211 (1993) 337
Dong, Z.-H., see Y. Wang 211 (1993) 341
Donley, E.A. and D.P. Shelton, Hyperpolarizabilities measured for interacting molecular pairs 215 (1993) 156
Donohue, D.L., see L.D. Hulett Jr. 216 (1993) 236
Donovan, R.J., see M.C.R. Cockett 214 (1993) 27
Donovan, R.J., see M.S.N. Al-Kahali 220 (1994) 225
Dorthe, G., see P. Caubet 218 (1994) 529
Douhal, A., F. Amat-Guerri, A.U. Acuña and K. Yoshihara, Picosecond vibrational relaxation in the excited-state proton-transfer of 2-(3′-hydroxy-2′-naphthyl)benzimidazole 217 (1994) 619
Douhal, A. and R. Sastre, Room-temperature triple proton transfer of 7-hydroxyquinoline and stabilization of its ground-state keto tautomer in a polymeric matrix 219 (1994) 91
Douhal, A., see F. Lahmani 220 (1994) 235
Douin, S., J.-H. Fillion, M. Bonneau, P. Bréchignac, D. Furio, D. Gauyacq, M. Horani and N. Shafizadeh, Dual time-of-flight photoelectron–photoion spectrometry on a magnetic bottle–molecular beam apparatus 216 (1993) 215
Dreier, T., see A.A. Suvernev 216 (1993) 1, 5
Dreizler, H., see H. Harder 214 (1993) 265
Dresselhaus, G., see J.M. Holden 220 (1994) 186
Dresselhaus, M.S., see J.M. Holden 220 (1994) 186
Dressler, R.A., S. Williams, S.T. Graul, R.H. Salter and E. Murad, Guided-ion beam measurements of the $Kr^+ + NO$ charge-transfer reaction 215 (1993) 656
Drickamer, H.G., see J.M. Lang 214 (1993) 310
Dubicki, L., see H. Riesen 218 (1994) 579
Dudis, D., see G.P. Das 212 (1993) 671
Dugourd, Ph., see K. Kobe 213 (1993) 554
Dugué, J., see B. Keita 215 (1993) 125
Dujardin, C., see C. Pédrini 220 (1994) 433
Dulles, F.J., see C.J. Cramer 218 (1994) 387
Dunbar, R.C. and J.D. Faulk, Radiative and collisional association of mesitylene ion with parent neutral at 196 K 214 (1993) 5

Duncan, J.L., see M.M. Law 212 (1993) 172
Duncan, M.A., see K.F. Willey 211 (1993) 156
Duplan, J.C., see L. Mahi 211 (1993) 27
Duppen, K., see E. Lenderink 211 (1993) 503
Dupré, P. and P.G. Green, Characterization of a large singlet–triplet coupling in the $\tilde{A}$ state of the acetylene molecule 212 (1993) 555
Durga Prasad, M., see V. Nagalakshmi 217 (1994) 279
Dusek, M., see J.L. de Boer 219 (1994) 469
Dusek, M., see M. Nikl 220 (1994) 14
Dutta, A.K., T.N. Misra and G.B. Talapatra, A Monte Carlo simulation of spectral diffusion in the presence of energetic and substitutional disorder 212 (1993) 637
Dutta, P., S. Adhikari and S.P. Bhattacharyya, Fourier grid Hamiltonian method for bound states of multidimensional systems. Formulation and preliminary applications to model systems 212 (1993) 677
Dyke, J.M., see J. Baker 213 (1993) 257
Dykstra, C.E., see J.D. Augspurger 213 (1993) 211
Dykstra, C.E., see K.A. Franken 220 (1994) 161
Dzuba, S.A., Y. Kodera, H. Hara and A. Kawamori, Dipolar interactions of spin probes in organic glasses studied by electron spin echo 214 (1993) 621

Eades, R.A., see C. Sosa 211 (1993) 265
Ebata, T., see S. Tanabe 215 (1993) 347
Ebbesen, T.W., see K. Tanigaki 213 (1993) 395
Eberhardt, W., see M. Neeb 212 (1993) 205
Eberhardt, W., see G. Ganteför 217 (1994) 600
Eckhoff, W.C., see D.L. Strout 214 (1993) 576
Eckhoff, W.C. and G.E. Scuseria, A theoretical study of the C_2 fragmentation energy of C_{60} and C_{70} 216 (1993) 399
Effantin, C., see R.F. Barrow 214 (1993) 293
Effenberger, F., see J. Walz 213 (1993) 321
Eggen, B.R., A.J. Marks, J.N. Murrell and S.C. Farantos, Water clusters – a speculation 219 (1994) 247
Egsgaard, H., see E.L. Thomsen 215 (1993) 257
Ehbrecht, M., M. Faerber, F. Rohmund, V.V. Smirnov, O. Stelmakh and F. Huisken, CO_2-laser-driven production of carbon clusters and fullerenes from the gas phase 214 (1993) 34
Eilers, H., U. Hömmerich, S.M. Jacobsen and W.M. Yen, The near-infrared emission of $Cr:Mn_2SiO_4$ and $Cr:MgCaSiO_4$ 212 (1993) 109
Eilers, H., see U. Hömmerich 213 (1993) 163
Eisenthal, K.B., see X. Zhao 214 (1993) 203
Eklund, P.C., see P. Zhou 211 (1993) 337
Eklund, P.C., see Y. Wang 211 (1993) 341; 217 (1994) 413
Eklund, P.C., see J.M. Holden 220 (1994) 186
El Ajli, M., see R. Stringat 220 (1994) 429
Eland, J.H.D., see T.A. Field 211 (1993) 436
Elguero, J., see O. Mó 219 (1994) 45
Ellermann, T., J. Sehested, O.J. Nielsen, P. Pagsberg and T.J. Wallington, Kinetics of the reaction of F atoms with O_2 and UV spectrum of FO_2 radicals in the gas phase at 295 K 218 (1994) 287
Ellert, Ch., see Th. Reiners 215 (1993) 357
Ellervee, A., see A. Freiberg 214 (1993) 10
El Misiery, A.M., see A.S. Shalabi 215 (1993) 275
Elvingson, C., Brownian dynamics simulations of DNA electric dichroism at high electric field strengths 214 (1993) 91
Emmel, M.D., see D. Farrelly 217 (1994) 520
Emsley, L., see R.G. Larsen 214 (1993) 220
Endo, Y., see Y. Ohshima 213 (1993) 95
Engdahl, C. and B.I. Lundqvist, Influence of the initial rotational state on the dissociation of hydrogen on copper 215 (1993) 103
Engel, H., see M. Braune 211 (1993) 534
Engel, V., see Ch. Meier 212 (1993) 691
Engel, W., see B. Rausenberger 215 (1993) 109
Engel, W., see M. Ondřejček 215 (1993) 528
Engert, C., S. Umapathy, W. Kiefer and H. Hamaguchi, Dynamic structure of charge carrier in polyaniline by near-infrared excited resonance Raman spectroscopy 218 (1994) 87
Enomoto, M., see J.S. Ahn 215 (1993) 336
Eriksson, L.A., J. Wang and R.J. Boyd, The effect of a neon matrix on the hyperfine structure of CH_4^+. A model study 211 (1993) 88
Eriksson, L.A., see J. Kong 217 (1994) 24

Erman, P., A. Karawajczyk, E. Rachlew-Källne, C. Strömholm, J. Larsson, A. Persson and R. Zerne, Direct determination of the ionization potential of CO by resonantly enhanced multiphoton ionization mass spectroscopy 215 (1993) 173
Ermler, W.C., see D. Andrae 220 (1994) 341
Ernst, H., D. Freude and I. Wolf, Multinuclear solid-state NMR studies of Brønsted sites in zeolites 212 (1993) 588
Ernst, M.C., A.F. Sax and J. Kalcher, Intramolecular H-transfer reactions in Si_2H_n (for $n=3$–5) 216 (1993) 189
Ernst, R.R., see S. Hediger 213 (1993) 627
Ernst, R.R., see M. Tomaselli 214 (1993) 1
Ertl, G., see H. Bludau 219 (1994) 452
Eryomin, V.V., see S.I. Vetchinkin 215 (1993) 11
Espinosa-Garcia, J. and J.C. Corchado, Theoretical values of the enthalpies of formation of the SH and HSO radicals 218 (1994) 128
Esquivel, R.O., see M. Hô 219 (1994) 15
Evans, J.E., see J.Z. Zhang 218 (1994) 479
Evleth, E.M., see F. Colonna 212 (1993) 665

Fabeni, P., see M. Nikl 220 (1994) 14
Fabre, C., see B. Keita 215 (1993) 125
Fabre, G., see R. Stringat 220 (1994) 429
Faerber, M., see M. Ehbrecht 214 (1993) 34
Fahlman, M., D. Beljonne, M. Lögdlund, R.H. Friend, A.B. Holmes, J.L. Brédas and W.R. Salaneck, Experimental and theoretical studies of the electronic structure of Na-doped poly(para-phenylenevinylene) 214 (1993) 327
Fain, B., T.C. Chang, H.T. Liou, D.Y. Yang, K.L. Huang, M.-C. Chan and S.H. Lin, Dual-frequency pump–probe time-resolved spectroscopy 216 (1993) 551
Fairbrother, D.H., see S.J. Garrett 219 (1994) 409
Falcetta, M.F. and P.E. Siska, Ab initio study of the long-range interaction between He^+ and H_2 213 (1993) 531
Fantucci, P., see V. Bonačić-Koutecký 213 (1993) 522
Farantos, S.C., see B.R. Eggen 219 (1994) 247
Fárník, M., Z. Dolejšek, Z. Herman and V.E. Bondybey, Beam scattering investigation of hydride-ion transfer processes. Reaction of CH_3^+ and CD_3^+ with C_2H_6 216 (1993) 458
Farrelly, D. and M.D. Emmel, Semiclassical quantization of doubly excited intrashell resonances of the helium atom 217 (1994) 520
Fassihi, M., see M. Rinnemo 211 (1993) 60
Fattori, V., see G. Giro 211 (1993) 580
Faulk, J.D., see R.C. Dunbar 214 (1993) 5
Feautrier, N., see A. Spielfiedel 216 (1993) 162
Fedrigo, S., W. Harbich, J. Belyaev and J. Buttet, Evidence for electronic shell structure of small silver clusters in the optical absorption spectra 211 (1993) 166
Fehér, M., A. Rohrbacher, J.P. Maier and A. Miklós, Optoacoustic spectroscopy of short-lived molecules 211 (1993) 171
Fehér, M., see T. Pasinszki 215 (1993) 395
Fehér, M. and P.A. Martin, Ab initio calculations of the properties of NO^+ in its ground electronic state $X\ ^1\Sigma$ 215 (1993) 565
Feldchtein, F., see S. Hess 216 (1993) 247
Felder, P., see M.-A. Thelen 213 (1993) 275
Felder, P., X. Yang and J.R. Huber, Photodissociation of nitric acid in a cold molecular beam at 193 nm 215 (1993) 221
Felder, P., see G.P. Morley 219 (1994) 195
Feldhaus, J., see M. Neeb 212 (1993) 205
Feldmann, T., see M. Cohen 218 (1994) 147
Feliu, J.M., see S. Remita 218 (1994) 115
Felps, S., see U. Asaf 212 (1993) 326
Fenet, B., see L. Mahi 211 (1993) 27
Feng, D., see S. Feng 214 (1993) 97
Feng, P.Y., see K. Balasubramanian 214 (1993) 85
Feng, S., D. Feng and C. Deng, Theoretical studies on the structures and reactivity of silylenoids. III. The structures and isomerization of silylenoid H_2SiNaF 214 (1993) 97
Fenistein, S., see S. Jullien 212 (1993) 340
Fernández, A. and A. Belinky, Learning to fold a random RNA chain 212 (1993) 201
Fernández-Serra, P., see V. Botella 219 (1994) 497
Ferrari, A.M., E. Garrone and P. Ugliengo, Ab initio study of the gas-phase equilibrium between $(H_2O)_4$ and $(H_2O)_8$ 212 (1993) 644

Ferrarini, A., G.R. Luckhurst, P.L. Nordio and S.J. Roskilly, Understanding the unusual transitional behaviour of liquid crystal dimers 214 (1993) 409
Ferrario, M., M.L. Klein and I.R. McDonald, Dynamical behavior of the azide ion in protic solvents 213 (1993) 537
Ferrero, J.C., see R.A. Bollati 218 (1994) 159
Ferretti, A. and A. Lami, Optical properties of pyrazine-bridged ruthenium chains by the two-band Hubbard Hamiltonian 220 (1994) 327
Feyereisen, M.W., see O. Vahtras 213 (1993) 514
Fichou, D., see J.-M. Nunzi 215 (1993) 114
Fiedler, A., J. Hrušák, W. Koch and H. Schwarz, The energetical and structural properties of FeO^+. An application of multireference perturbation theory 211 (1993) 242
Field, R.W., see R. Liyanage 216 (1993) 544
Field, R.W., see G.M. Schmid 219 (1994) 331
Field, T.A. and J.H.D. Eland, Lifetimes of metastable molecular doubly charged ions 211 (1993) 436
Figari, G., see V. Magnasco 213 (1993) 17
Figuera, J.M., see M. Castillejo 214 (1993) 227
Fillion, J.-H., see S. Douin 216 (1993) 215
Fink, E.H., see O. Shestakov 211 (1993) 473
Fink, E.H., see R. Breidohr 218 (1994) 13
Finney, L.M., A. Borrmann and C.C. Martens, Nonstationary time series analysis of intramolecular energy transfer 214 (1993) 159
Finnila, A.B., M.A. Gomez, C. Sebenik, C. Stenson and J.D. Doll, Quantum annealing: a new method for minimizing multidimensional functions 219 (1994) 343
Fiorini, C., see J.-M. Nunzi 219 (1994) 349
Fiory, A.T., see R.C. Haddon 218 (1994) 100
Fischer, P.R., J.L. Daschbach and G.L. Richmond, Surface second harmonic studies of Si(111)/electrolyte and Si(111)/SiO_2/electrolyte interfaces 218 (1994) 200
Fitzgerald, G., see C. Sosa 211 (1993) 265
Fleissner, G., A. Hallbrucker and E. Mayer, Raman spectroscopic evidence for increasing contact-ion pairing in the glassy states of "dilute" aqueous calcium nitrate solutions 218 (1994) 93
Fletcher, J., see P. Bond 211 (1993) 649
Fletcher, T.R., see K. Ravichandran 217 (1994) 375
Flügge, J., see P. Botschwina 215 (1993) 681
Fockenberg, Ch., H. Saathoff and R. Zellner, A laser photolysis/LIF study of the rate constant for the reaction $CF_3O+O_3 \rightarrow$ products 218 (1994) 21
Foggi, P., see C. Taiti 212 (1993) 283
Folden, C.A., see A.T. Balaban 217 (1994) 266
Foltin, M., see M. Kolibiar 219 (1994) 252
Ford, J.V., see Z. Shi 220 (1994) 274
Forest, S.E. and R.L. Kuczkowski, The microwave spectrum of cyclopropane·ammonia. A novel structure for cyclopropane complexes 218 (1994) 349
Forrest, S.R., see E.I. Haskal 219 (1994) 325
Fort, A., see M. Lequan 213 (1993) 71
Fortunelli, A. and A. Painelli, Interacting electrons in the solid state: the role of orbital relaxation 214 (1993) 402
Foss, M., F. Besenbacher, C. Klink and I. Stensgaard, Deuterium-induced restructuring of Cu(100) 215 (1993) 535

Fournier, T., see T.-H. Tran-Thi 213 (1993) 139
Fowler, G.J.S., see H. van der Laan 212 (1993) 569
Fowler, P.W., H.M. Kelly and A.J. Sadlej, Electric and magnetic properties of the phosphorus trifluoride molecule 212 (1993) 659
Fowler, P.W., H.M. Kelly and R.J.C. Brown, The nitrogen Sternheimer antishielding factor in the ammonium ion 216 (1993) 200
Fox, D.J., see B.G. Johnson 218 (1994) 595
Fraenkel, R. and Y. Haas, Photolysis of ICN in a cryogenic matrix 214 (1993) 234
Fraenkel, R. and Y. Haas, A molecular dynamics simulation of NBr trapping in an argon matrix 220 (1994) 77
Fragalà, I.L., see S. Di Bella 214 (1993) 598
Fraissard, J., see A. Gedeon 219 (1994) 440
Francisco, J.S., Z. Li, A. Bradley and A.E.W. Knight, Degradation of alternative halocarbons. Decomposition pathways of trifluoroethoxy radicals 214 (1993) 77
Francisco, J.S., Z. Li, M.R. Hand and I.H. Williams, Theoretical characterisation of the lowest $n\rightarrow\pi^*$ electronic state of CF_2O. Is it planar or non-planar? 214 (1993) 591
Francisco, J.S. and Y. Su, An ab initio study of the reaction between FO radicals and H_2O 215 (1993) 58
Francisco, J.S., see T.S. Dibble 215 (1993) 409, 423
Francisco, J.S. and Y. Su, A computational study of the reaction between FO radicals and methane 215 (1993) 417
Francisco, J.S., Ab initio investigation of the decomposition of trifluoromethanol into carbonyl fluoride and hydrogen fluoride 218 (1994) 401
Francisco, J.S., see J.A. Montgomery Jr. 220 (1994) 391
Franken, K.A. and C.E. Dykstra, Quantum Monte Carlo vibrational analysis of the nitrogen–water complex 220 (1994) 161
Frankevich, E., Y. Maruyama and H. Ogata, Mobility of charge carriers in vapor-phase grown C_{60} single crystal 214 (1993) 39
Frankevich, E.L., see M.M. Triebel 214 (1993) 315, 321
Frantsuzov, P.A., see A.A. Zharikov 220 (1994) 319
Frederick, J.H., see V.D. Vachev 215 (1993) 306
Freeman, R., see V. Blechta 215 (1993) 341
Frei, G., see C.P.M. Giesbergen 213 (1993) 597
Freiberg, A., A. Ellervee, P. Kukk, A. Laisaar, M. Tars and K. Timpmann, Pressure effects on spectra of photosynthetic light-harvesting pigment–protein complexes 214 (1993) 10
Freiser, B.S., see S. Afzaal 218 (1994) 254
Frens, A.M., see M. Matsushita 214 (1993) 349
Freude, D., see H. Ernst 212 (1993) 588
Fricke, B., see T. Baştuğ 211 (1993) 119
Friedrich, K.A. and G.L. Richmond, Surface second harmonic generation studies of stepped Ag(111) electrode surfaces 213 (1993) 491
Friend, R.H., see I.D.W. Samuel 213 (1993) 472
Friend, R.H., see M. Fahlman 214 (1993) 327
Frisch, M.J., see B.G. Johnson 216 (1993) 133
Frish, M., see R.R. Pappalardo 212 (1993) 12
Fuchs, A.H., see F.M. Bénière 215 (1993) 301
Fuchs, A.H., see A. Boutin 218 (1994) 122
Fuchs, C., see V. Bonačić-Koutecký 213 (1993) 522

Fuentealba, P. and A. Savin, A test for the Wilson–Levy correlation energy functional 217 (1994) 566
Fuglesang, C.D., see D.A. Baugh 219 (1994) 207
Fujii, M., see S. Tanabe 215 (1993) 347
Fujimoto, N., see Y. Saito 212 (1993) 379
Fujitani, Y., T. Miyazaki, N.M. Masaki, Y. Aratono and E. Tachikawa, Effect of rotational quantum states ($J=0, 1$) on the tunneling reaction $H_2+T\rightarrow H+HT$ in xenon–hydrogen mixtures at 77 K 214 (1993) 301
Fujito, T., see T. Fujiwara 212 (1993) 81
Fujiwara, T., A. Ramamoorthy, K. Nagayama, K. Hioka and T. Fujito, Dipolar HOHAHA under MAS conditions for solid-state NMR 212 (1993) 81
Fujiwara, Y., see H. Mukaihata 211 (1993) 140
Fujiwara, Y., M. Mukai, T. Tamura, Y. Tanimoto and M. Okazaki, A laser flash photolysis study of the effect of intense magnetic fields on the photoreaction of benzophenone in SDS micellar solution 213 (1993) 89
Fujiwara, Y., see R. Takasu 217 (1994) 478
Fukazawa, N., see S. Yamamoto 215 (1993) 323
Fukazawa, N., see S. Hashimoto 219 (1994) 445
Fukazawa, N., H. Fukumura, H. Masuhara and J. Prochorow, A picosecond diffuse reflectance laser photolysis study on phenanthrene–pyromellitic dianhydride charge-transfer crystal 220 (1994) 461
Fuke, K., see H. Umemoto 214 (1993) 271
Fukumura, H., see S. Yamamoto 215 (1993) 323
Fukumura, H., see S. Hashimoto 219 (1994) 445
Fukumura, H., see N. Fukazawa 220 (1994) 461
Fulara, J., M. Jakobi and J.P. Maier, Electronic and infrared spectra of C_{60}^+ and C_{60}^- in neon and argon matrices 211 (1993) 227
Fulde, P., see J. Gräfenstein 215 (1993) 611
Fülscher, M., see L. Serrano-Andrés 211 (1993) 125
Furio, D., see S. Douin 216 (1993) 215
Furlani, A., see G. Polzonetti 214 (1993) 333
Furuuchi, H., see T. Arai 212 (1993) 597
Furuya, Y., see T. Arai 212 (1993) 597

Gadonas, R., see R. Gagel 217 (1994) 228
Gadre, S.R. and R.N. Shirsat, Comment on "Computing molecular electrostatic potentials with the PRISM algorithm" 218 (1994) 593
Gagel, R., R. Gadonas and A. Laubereau, Evidence for biexcitons and dynamic Stark effect in J-aggregates from femtosecond spectroscopy 217 (1994) 228
Gale, J.D., C.R.A. Catlow and J.R. Carruthers, An ab initio study of methanol adsorption in zeolites 216 (1993) 155
Gallazzi, A.M., see M. Nisoli 220 (1994) 64
Gal'pern, E.G., I.V. Stankevich, A.L. Chistykov and L.A. Chernozatonskii, Carbon nanotubes with metal inside: electron structure of tubelenes $[Li@C_{24}]_n$ and $[K@C_{36}]_n$ 214 (1993) 345
Galvão, D.S., see R.H. Baughman 211 (1993) 110
Ganguly, B., see S.P. Ananthavel 217 (1994) 101
Ganteför, G. and W. Eberhardt, Shell structure and s–p hybridization in small aluminum clusters 217 (1994) 600
García, F., see G.G. Lazarev 212 (1993) 319
García de la Vega, J.M. and B. Miguel, Single-exponent Slater function expansions of the He atom is orbital and its isoelectronic series (Chem. Phys. Letters 207 (1993) 270). Erratum 212 (1993) 420
García Solé, J., see U. Caldiño G. 213 (1993) 84
García-Sucre, M., see J.L. Paz 217 (1994) 333
Gardner, J.A., see T.L. Thiem 218 (1994) 309
Garofalini, S.H., see S. Blonski 211 (1993) 575
Garofalini , S.H., see F. Liu 215 (1993) 401
Garrett, S.J., D.H. Fairbrother, V.P. Holbert, E. Weitz and P.C. Stair, Multiphoton ionization mechanisms in CH_3I and CD_3I 219 (1994) 409
Garrett, W.R., see R.B. Jones 212 (1993) 451
Garrone, E., see A.M. Ferrari 212 (1993) 644
Gartstein, Yu.N. and E.M. Conwell, High-field hopping mobility of polarons in disordered molecular solids. A Monte Carlo study 217 (1994) 41
Gasparoli, A., see G. Karwasz 211 (1993) 529
Gatti, C., see V. Bonačić-Koutecký 213 (1993) 522
Gauyacq, D., see S. Douin 216 (1993) 215
Gburski, Z.E., see H. Stassen 217 (1994) 325
Ge, M. and K. Sattler, Observation of fullerene cones 220 (1994) 192
Gedanken, A., see E. Sominska 213 (1993) 117
Gedeon, A. and J. Fraissard, ^{129}Xe NMR of AgX, CuX, ZnX and CdX zeolites. Comparative study of nd^{10} element–xenon interactions 219 (1994) 440
Geen, H., J.J. Titman and H.W. Spiess, Heteronuclear magnetization transfer in rapidly spinning solids 213 (1993) 145
Geerlings, P., see F. de Proft 220 (1994) 405
Gehlen, M.H., Fluorescence quenching in clusters of reverse micelles 212 (1993) 362
Geil, B. and G. Hinze, Influence of data treatment on the shape of ^2H NMR T_1 curves 216 (1993) 51
Gejo, T., M. Takayanagi, T. Kono and I. Hanazaki, Photodissociation dynamics of acetaldehyde. Vibrational energy distribution in the photofragment HCO 218 (1994) 343
Gelb, L.D. and R.M. Lynden-Bell, Force oscillations and liquid structure in simulations of an atomic force microscope tip in a liquid 211 (1993) 328
George, S.M., see D.R. Haynes 214 (1993) 50

George, T.F., see I. Last 216 (1993) 599
Gerber, Ch., see J.K. Gimzewski 213 (1993) 401; 217 (1994) 589
Gertner, I., see I. Ben-Itzhak 212 (1993) 467
Ghose, K.B., P.G. Nair and S. Pal, Implementation of a stationary coupled-cluster response method 211 (1993) 15
Ghosh, A. and J. Almlöf, The ultraviolet photoelectron spectrum of free-base porphyrin revisited. The performance of local density functional theory 213 (1993) 519
Ghosh, T.K., A.K. Das and P.K. Mukherjee, New resonances in a dynamic polarizability calculation 218 (1994) 433
Gibbons, V.C., see J. Baker 215 (1993) 163
Gierer, M., see H. Bludau 219 (1994) 452
Giesbergen, C.P.M., C. Terletski, G. Frei, H.U. Güdel and M. Glasbeek, Optically detected magnetic resonance spectroscopy of rhodium(III) mixed-chelate complexes 213 (1993) 597
Gilbert, J.V., A.M. Zarubaiko and S. Lantz, UV absorption spectrum of low-temperature matrix-isolated NFCl radicals 220 (1994) 19
Gildemeister, J.M. and G.K. Wertheim, Electronic properties of Cs_xC_{60} films for the complete range of stoichiometries 220 (1994) 181
Gilibert, M., see A. Aguilar 220 (1994) 267
Gill, D., see Z. Chernia 212 (1993) 57
Gill, P.M.W., see K. Raghavachari 214 (1993) 357; 220 (1994) 385
Gill, P.M.W., B.G. Johnson and J.A. Pople, A simple yet powerful upper bound for Coulomb integrals 217 (1994) 65
Gill, P.M.W., see B.G. Johnson 218 (1994) 595; 220 (1994) 377
Gillan, M.J., see I. Štich 212 (1993) 617
Gillbro, T., see S.M. Bachilo 218 (1994) 557
Giménez, X., see A. Aguilar 220 (1994) 267
Gimzewski, J.K., S. Modesti, Ch. Gerber and R.R. Schlittler, Observation of a new Au(111) reconstruction at the interface of an adsorbed C_{60} overlayer 213 (1993) 401
Gimzewski, J.K., Ch. Gerber, E. Meyer and R.R. Schlittler, Observation of a chemical reaction using a micromechanical sensor 217 (1994) 589
Giro, G., J. Kalinowski, P.D. Marco, V. Fattori and G. Marconi, Absorption tail photoconductivity in solid films of C_{60} 211 (1993) 580
Glasbeek, M., see C.P.M. Giesbergen 213 (1993) 597
Głaz, W., J. Yang, J.D. Poll and C.G. Gray, Complex plane method for interaction-induced spectra in 3D systems 218 (1994) 183
Glish, G.L., see L.D. Hulett Jr. 216 (1993) 236
Goddard, J.D., see C.G. Joslin 213 (1993) 377
Goldanskii, V.I. and F. Parak, Some still open questions of relaxational CO–heme rebinding 219 (1994) 379
Goldberg, N., D. Sülzle and H. Schwarz, The gas-phase generation and characterization of butatrienylidene H_2CCCC: by neutralization–reionization mass spectrometry 213 (1993) 593
Goldman, S., see C.G. Joslin 211 (1993) 587; 213 (1993) 377; 215 (1993) 144
Gomez, M.A., see A.B. Finnila 219 (1994) 343
Gong, M., Y. Bao, R.S. Urdahl and W.M. Jackson, LIF measurements of radiative lifetimes of the $C_2(B'\,^1\Sigma_g^+)$ state 217 (1994) 210
Gong, M.-X., see R. Huang 216 (1993) 108, 115
González, M., see A. Aguilar 220 (1994) 267
Goo, J.S., see K. Lee 216 (1993) 483

Goode, J.G., see M.C.R. Cockett 214 (1993) 27
Göpel, W., see P. Lemoine 220 (1994) 177
Gorbunov, B.Z., E.L. Zapadinsky, K.K. Sabelfeld and M. Ataev, Influence of inhomogeneity and fluctuations of supersaturation on heterogeneous nucleation 215 (1993) 31
Gordon, E.B., V.V. Khmelenko and O.S. Rzhevsky, Critical phenomena in electron drift through condensed rare gases 217 (1994) 605
Gordon, M.S., see T.L. Windus 216 (1993) 375
Gordon, R.D., J. Michael Hollas, P.J.A. Ribeiro-Claro and J.J.C. Teixeira-Dias, CF_3-torsional potentials of 2-aminobenzotrifluoride in the S_0 and S_1 electronic states from fluorescence spectra in a supersonic jet 211 (1993) 392
Gordon, R.J., see R. Liyanage 216 (1993) 544
Gorry, P.A., see P. Bond 211 (1993) 649
Gorse, C., see G. Colonna 213 (1993) 5
Gosine, J.N., see X. Song 217 (1994) 216
Goto, M. and S. Saito, Submillimeter-wave spectra of the PH and PD radicals in the $^3\Sigma^-$ state 211 (1993) 443
Gotschy, B., see A. Skiebe 220 (1994) 138
Gotts, N.G., see G. von Helden 212 (1993) 241
Goubert, L., G.D. Billing, E. Desoppere and W. Wieme, Semiclassical calculation of the probabilities for collision-induced vibrational transitions in Ar_2^* 219 (1994) 360
Govoni, D.E., J.A. Booze, A. Sinha and F.F. Crim, The non-resonant signal in laser-induced grating spectroscopy of gases 216 (1993) 525
Goyal, P.S., S.V.G. Menon, B.A. Dasannacharya and V. Rajagopalan, Role of van der Waals forces on small angle neutron scattering from ionic micellar solutions 211 (1993) 559
Grabmaier, B.C., see E. Bayer 216 (1993) 228
Graener, H., see K. Wolfrum 213 (1993) 41
Gräfenstein, J., H. Stoll and P. Fulde, Computation of the valence band of diamond by means of local increments 215 (1993) 611
Graja, A., see N.D. Kushch 215 (1993) 137
Graul, S.T., see R.A. Dressler 215 (1993) 656
Gray, C.G., see C.G. Joslin 211 (1993) 587; 213 (1993) 377; 215 (1993) 144
Gray, C.G., see W. Głaz 218 (1994) 183
Gray, C.G., see A.R. Denton 219 (1994) 310
Gray, J.A. and R. Trebino, Two-photon-resonant four-wave-mixing spectroscopy of atomic hydrogen in flames 216 (1993) 519
Grayson, M. and W.T. Raynes, Electric field effects on the magnetic shielding of first and second row nuclei in some simple molecules 214 (1993) 473
Grayson, M. and W.T. Raynes, Electric field effects on proton magnetic shielding in some binary hydrides 218 (1994) 270
Grebner, D., see D.V. Lap 211 (1993) 135
Green, P.G., see P. Dupré 212 (1993) 555
Greenlief, C.M., see L.A. Keeling 217 (1994) 136
Gregori, A., see A. De Santis 213 (1993) 239
Grein, F., see A.B. Sannigrahi 214 (1993) 609
Grimley, T.B., The quantum theory of the rates of sticking and desorption 214 (1993) 447
Grimme, S., S.D. Peyerimhoff, S. Bartram, F. Vögtle, A. Breest and J. Hormes, Experimental and theoretical study of the circular dichroism spectra of oxa- and thia-[2.2]metacyclophane 213 (1993) 32

Grinberg, O.Ya., see S.D. Chemerisov 218 (1994) 353
Grishanin, B.A., see V.D. Vachev 215 (1993) 306
Groenen, E.J.J., see M. Matsushita 214 (1993) 349
Groombridge, C.J., see P.J. Barrie 219 (1994) 491
Gross, H., Y. He, M. Quack, A. Schmid and G. Seyfang, Time-resolved detection of reaction products in the infrared laser chemistry of sulfoxides: C_2H_4SO, $(CH_3)_2SO$, $(CD_3)_2SO$ 213 (1993) 122
Grunze, M., see Ch. Zubrägel 219 (1994) 127
Gryziński, M., Dynamical model of the molecular bond 217 (1994) 481
Gu, X., L.A. Muñoz, Y. Ishikawa and B.R. Weiner, Isotope effects and wavelength dependence in the rotational state distributions of the diatomic photofragments SH and SD from the photodissociation of H_2S and D_2S 211 (1993) 65
Güdel, H.U., see C.P.M. Giesbergen 213 (1993) 597
Guillaud, G. and J. Simon, Transient properties of nickel phthalocyanine thin film transistors 219 (1994) 123
Guillotin, J.-P., see R. Azria 220 (1994) 417
Guo, H., see M.H.M. Janssen 214 (1993) 281
Guo, H., L. Liu and K. Lao, Non-perturbative time-dependent quantal dynamics of superexchange in electron transfer processes 218 (1994) 212
Guo, J., see X. Mao 218 (1994) 249
Gurav, A.S., T.T. Kodas, L.-M. Wang, E.I. Kauppinen and J. Joutsensaari, Generation of nanometer-size fullerene particles via vapor condensation 218 (1994) 304
Gurioli, M., see M. Nikl 220 (1994) 14
Gustavsson, T., see P. Hébert 213 (1993) 345
Gütlich, P., see Th. Buchen 220 (1994) 262
Gutman, I., D. Todorović and M. Vučković, A variant of the Frank chiral amplification model 216 (1993) 447
Gutman, I., J. Brunvoll, B.N. Cyvin, E. Brendsdal and S.J. Cyvin, Essentially disconnected fully-acenoids, and fully-arenoid hydrocarbons 219 (1994) 355
Güttler, F., see M. Croci 212 (1993) 71
Güttler, F., T. Irngartinger, T. Plakhotnik, A. Renn and U.P. Wild, Fluorescence microscopy of single molecules 217 (1994) 393
Gvishi, R., R. Reisfeld and Z. Burshtein, Excited-state absorption in red perylimide dye in solution 212 (1993) 463
Gvishi, R., R. Reisfeld and Z. Burshtein, Spectroscopy and laser action of the "red perylimide dye" in various solvents 213 (1993) 338

Haaland, P.D., see J. Holtgrave 215 (1993) 548
Haarer, D., see R.B. Altmann 216 (1993) 281
Haas, Y., see R. Fraenkel 214 (1993) 234; 220 (1994) 77
Haberland, H., see Th. Reiners 215 (1993) 357
Habu, M., see H. Sekiya 215 (1993) 641
Hackett, P.A., see K. Athanassenas 213 (1993) 105
Haddon, R.C., A.S. Perel, R.C. Morris, S.-H. Chang, A.T. Fiory, A.F. Hebard, T.T.M. Palstra and G.P. Kochanski, Electrical resistivity and stoichiometry of K_xC_{60}, Rb_xC_{60}, and Cs_xC_{60} films 218 (1994) 100
Haffer, C.M. and M. Kunst, Computational simulations of charge carrier kinetics in a-Si:H 211 (1993) 203
Hagler, T.W., Nonparallel transition dipole moments and the polarization dependence of electroabsorption in nonoriented conjugated polymer films 218 (1994) 195
Hähner, G., see Ch. Zubrägel 219 (1994) 127
Hall, J., O. Saksager and I. Chorkendorff, Dissociative chemisorption of O_2 on Cu(100). Effects of mechanical energy transfer and recoil 216 (1993) 413
Hall, R.J., N.A. Burton, I.H. Hillier and P.E. Young, Tautomeric equilibria in 2-hydroxypyridine and in cytosine. An assessment of density functional methods, including gradient corrections 220 (1994) 129
Hallbrucker, A., see G. Fleissner 218 (1994) 93
Halonen, L., see M. Saarinen 219 (1994) 181
Halvick, P., see L. Bonnet 216 (1993) 11
Halvorson, C., R. Wu, D. Moses, F. Wudl and A.J. Heeger, Third harmonic generation spectra of degenerate ground state derivatives of poly(1,6-heptadiyne) 212 (1993) 85
Halvorson, C. and A.J. Heeger, Two-photon absorption spectrum of oriented trans-polyacetylene 216 (1993) 488
Hamaguchi, H., see T. Tahara 217 (1994) 369
Hamaguchi, H., see C. Engert 218 (1994) 87
Hamai, S., N. Tamai and H. Masuhara, Effects of the solid/liquid interface on the excimer formation of pyrene in toluene containing poly(methyl methacrylate). A time-resolved total internal reflection fluorescence study 213 (1993) 407
Hamanoue, K., see T. Nakayama 213 (1993) 581; 215 (1993) 622; 220 (1994) 219
Hamilton, P.A., see J. Baker 213 (1993) 297; 215 (1993) 163
Hammerich, A.D., see U. Manthe 211 (1993) 7
Hammonds, K.D., I.R. McDonald and J.-P. Ryckaert, Conformer distribution and the kinetics of trans–gauche isomerization in a model of liquid *n*-octane 213 (1993) 27
Han, K.-L., see R.-J. Li 220 (1994) 281
Hanazaki, I., see Y. Mori 211 (1993) 421
Hanazaki, I., Fragment rotational excitation due to the parent rotation in the dissociation of molecules 218 (1994) 151
Hanazaki, I., see T. Gejo 218 (1994) 343
Hanazaki, I., see T. Sekiguchi 219 (1994) 81
Hand, M.R., see J.S. Francisco 214 (1993) 591
Handa, Y.P., see J.S. Tse 215 (1993) 383
Handy, N.C., see C. Schmidt 211 (1993) 272
Handy, N.C., see S.M. Colwell 217 (1994) 271
Haneman, D. and H. Tributsch, d-state contribution to STM. Structure of van der Waals surfaces ($TaSe_2$, $Mo_{0.5}W_{0.5}Se_2$) and relevance for catalysis 216 (1993) 81

Hansen, K., C. Yeretzian and R.L. Whetten, A simple rate equation for fullerene coalescence 218 (1994) 462
Hara, H., see S.A. Dzuba 214 (1993) 621
Harbich, W., see S. Fedrigo 211 (1993) 166
Harbola, M.K., Electric dipole polarizabilities for helium-like ions from correlated wavefunctions. A density-functional approach 217 (1994) 461
Harcourt, R.D., Valence bond studies of the barrier to rotation around the N–N bond of N_2O_4 218 (1994) 175
Harder, H., H.-W. Nicolaisen, H. Dreizler and H. Mäder, One- and two-dimensional Fourier transform spectroscopy in the microwave and radiofrequency range of trifluoromethane in the vibrational state $v_6=1$ 214 (1993) 265
Hartke, B. and E.A. Carter, Ab initio molecular dynamics simulated annealing at the generalized valence bond level. Application to a small nickel cluster 216 (1993) 324
Hase, H. and Y. Miyatake, Electronic spectra of C_{70} anions produced in γ-irradiated organic glasses at 77 K 215 (1993) 141
Haselbach, E., see E. Vauthey 215 (1993) 264
Hashimoto, S., N. Fukazawa, H. Fukumura and H. Masuhara, Observation and characterization of excimer emission from anthracene included in NaX zeolite 219 (1994) 445
Hashizume, T., see Y. Kohno 214 (1993) 603
Hashizume, T., see X.-D. Wang 216 (1993) 409
Haskal, E.I., Y. Zhang, P.E. Burrows and S.R. Forrest, Finite size effects observed in the fluorescence of ultrathin crystalline organic films grown by organic molecular beam deposition 219 (1994) 325
Hasselbrink, E., see K.W. Kolasinski 219 (1994) 113
Hatherly, P.A., see D.M. Smith 216 (1993) 493
Hatta, N. and K. Murata, Very long graphitic nano-tubules synthesized by plasma-decomposition of benzene 217 (1994) 398
Hättig, C., see J.G. Ángyán 219 (1994) 267
Haugen, H.K., see L.H. Andersen 217 (1994) 204
Havenith, M., see G. Hilpert 219 (1994) 384
Hayashi, H., see M. Wakasa 215 (1993) 631
Hayashi, H., see Y. Nakamura 217 (1994) 387
Hayashi, K., see M. Yagi 211 (1993) 179
Hayashi, M., R. Islampour and S.H. Lin, The calculation of single-vibronic level rate constants for displaced-distorted potential surfaces 213 (1993) 465
Hayden, B.E., see A.E. Wiskerke 216 (1993) 93
Hayden, B.E., see D.A. Butler 217 (1994) 423
Haynes, D.R., A. Tokmakoff and S.M. George, Temperature-dependent absolute fluorescence quantum yield of C_{60} multilayers 214 (1993) 50
He, G., see G. Ding 220 (1994) 1
He, G.-Z., see R.-J. Li 220 (1994) 281
He, Y., see H. Gross 213 (1993) 122
He, Y., M. Quack, R. Ranz and G. Seyfang, Diode laser detection of iodine atom hyperfine transitions during and after infrared multiphoton excitation and dissociation of CF_3I with short pulse CO_2 lasers 215 (1993) 228
Head, J.D. and S. Jin, Efficient tools for theoretically investigating surface structure applied to Al on graphite 212 (1993) 32
Head-Gordon, M., see R.J. Rico 213 (1993) 224; 218 (1994) 139

Head-Gordon, M., R.J. Rico, M. Oumi and T.J. Lee, A doubles correction to electronic excited states from configuration interaction in the space of single substitutions 219 (1994) 21
Head-Gordon, M. and T. Head-Gordon, Analytic MP2 frequencies without fifth-order storage. Theory and application to bifurcated hydrogen bonds in the water hexamer 220 (1994) 122
Head-Gordon, T., see M. Head-Gordon 220 (1994) 122
Hebard, A.F., see R.C. Haddon 218 (1994) 100
Heber, O., see I. Ben-Itzhak 212 (1993) 467
Hébert, P., G. Baldacchino, T. Gustavsson and J.-C. Mialocq, Sub-picosecond fluorescence study of the LDS 751 dye molecule in ethanol 213 (1993) 345
Hediger, S., B.H. Meier and R.R. Ernst, Cross polarization under fast magic angle sample spinning using amplitude-modulated spin-lock sequences 213 (1993) 627
Heeger, A.J., see C. Halvorson 212 (1993) 85; 216 (1993) 488
Heeger, A.J., see B. Kraabel 213 (1993) 389
Heeger, A.J., see J.L. Brédas 217 (1994) 507
Hegazi, E., see J. Supronowicz 218 (1994) 240
Hegde, M.S., see S.P. Ananthavel 217 (1994) 101
Heinemann, C. and W. Thiel, Ab initio study on the stability of diaminocarbenes 217 (1994) 11
Heinemann, D., see T. Baştuğ 211 (1993) 119
Heinzel, C., see E. Rühl 211 (1993) 403
Helenius, V., see E. Laitinen 218 (1994) 73
Helgaker, T., see M. Jaszunski 220 (1994) 154
Henderson, C.C., C.M. Rohlfing and P.A. Cahill, Theoretical studies of selected $C_{60}H_2$ and $C_{70}H_2$ isomers 213 (1993) 383
Henderson, D., see W. Schmickler 216 (1993) 424
Heninger, M., see S. Jullien 212 (1993) 340
Henriksen, N.E. and B. Amstrup, Coherent control of HOD photodissociation dynamics in the first absorption band 213 (1993) 65
Hepburn, J.W., see A. Mank 219 (1994) 169
Herbert, L.B., see I.R. Sims 211 (1993) 461
Herbst, E., see S.A. Maluendes 217 (1994) 571
Herman, Z., see M. Fárník 216 (1993) 458
Herman, Z., see C. Berg 216 (1993) 465
Hermant, R.M., see S. Depaemelaere 215 (1993) 649
Hernandez, R. and W.H. Miller, Semiclassical transition state theory. A new perspective 214 (1993) 129
Herrero, C.P., Framework dependence of atom ordering in tectosilicates. A lattice gas model 215 (1993) 587
Herrero, V.J., see F.J. Aoiz 211 (1993) 72; 218 (1994) 422
Herreros, B. and J. Klinowski, Synthesis of zeolites from sodium silicoglycolate, a 5-coordinate silicon compound 220 (1994) 478
Hershberger, J.F., see J. Park 218 (1994) 537
Hertel, N., see L.H. Andersen 217 (1994) 204
Hese, A., see M. Okruss 220 (1994) 286
Hess, B.A., see G. Jansen 214 (1993) 103
Hess, B.A., see P. Schwerdtfeger 218 (1994) 362
Heß, B.A., see J.G. Ángyán 219 (1994) 267
Heß, B.A., see K. Dietz 220 (1994) 397
Hess, S., F. Feldchtein, A. Babin, I. Nurgaleev, T. Pullerits, A. Sergeev and V. Sundström, Femtosecond energy transfer within the LH2 peripheral antenna of the photosynthetic purple bacteria *Rhodobacter sphaeroides* and *Rhodopseudomonas palustris* LL 216 (1993) 247

Heully, J.-L., see D. Maynau 211 (1993) 625
Heully, J.L., see J. Meller 218 (1994) 276
Heyl, Ä., see P. Botschwina 215 (1993) 681
Higgins, D.A., R.R. Naujok and R.M. Corn , Second harmonic generation measurements of molecular orientation and coadsorption at the interface between two immiscible electrolyte solutions 213 (1993) 485
Higo, J., see T. Yamato 219 (1994) 155
Higuchi, J., see M. Yagi 211 (1993) 179
Hill, J.-R., see J. Sauer 218 (1994) 333
Hillier, I.H., see P.E. Young 215 (1993) 405
Hillier, I.H., see R.J. Hall 220 (1994) 129
Hilpert, G., H. Linnartz, M. Havenith, J.J. ter Meulen and W.L. Meerts, Tunable infrared and far-infrared direct absorption spectroscopy of molecular ions in a supersonic jet expansion 219 (1994) 384
Hinchliffe, A. and H.J. Soscun Machado, Ab initio study of the static dipole polarizability of naphthalene 214 (1993) 64
Hinek, M.J., see J. Supronowicz 213 (1993) 282
Hinek, M.J., see W. Kedzierski 218 (1994) 314
Hintsa, E.J., see W. Sun 218 (1994) 515
Hinze, G., see B. Geil 216 (1993) 51
Hioka, K., see T. Fujiwara 212 (1993) 81
Hirata, F., see S. Ten-no 214 (1993) 391
Hirosawa, I., see K. Tanigaki 213 (1993) 395
Hirose, C., see S. Sekine 212 (1993) 129
Hirota, N., see M. Terazima 214 (1993) 541
Hirsch, A., see A. Skiebe 220 (1994) 138
Hirsch, G., see Y. Li 212 (1993) 185
Hirsch, G., see H.-P. Liebermann 214 (1993) 381
Hiyama, M. and S. Iwata, Theoretical assignment of the vibronic bands in the photoelectron spectra of N_2 below 30 eV 211 (1993) 319
Ho, K.M., see X.Q. Wang 214 (1993) 193; 217 (1994) 199
Hồ, M., R.P. Sagar, J.M. Pérez-Jordá, V.H. Smith Jr. and R.O. Esquivel, A numerical study of molecular information entropies 219 (1994) 15
Hobza, P., see J. Vacek 220 (1994) 85
Hochstrasser, R.M., see J.P. Culver 214 (1993) 431
Hoeft, J. and T. Törring, The microwave rotational spectrum of X $^2\Sigma^+$ YO 215 (1993) 367
Hoeft, J. and K.P.R. Nair, Millimeter wave rotational spectrum of gallium monofluoride 215 (1993) 371
Hof, M., see H. Lanig 220 (1994) 423
Hoffman, D.K., see Y. Huang 213 (1993) 209; 214 (1993) 451
Hoffman, D.K., see W. Zhu 217 (1994) 73
Hoffman, D.K., see D.J. Kouri 220 (1994) 312
Hoffmann, E. and A. Schweiger, Stimulated echo description of coherent Raman beat EPR spectroscopy 220 (1994) 467
Hoffmann, H., see K.L. Walther 212 (1993) 96
Hofmann, H.-J., see R. Cimiraglia 217 (1994) 430
Hogreve, H., The ground state geometry of the Ne_3^+ trimer 215 (1993) 72
Hohm, U., Modelling of the long-range part of the invariants of the incremental pair polarizability tensor $\Delta\hat{\alpha}$ 211 (1993) 498

Hohmann, J., G. Müller, G. Schönnenbeck and F. Stuhl, Temperature-dependent quenching of $O_2(b\ ^1\Sigma_g^+)$ by H_2, D_2, CO_2, HN_3, DN_3, HNCO and DNCO 217 (1994) 577
Holbert, V.P., see S.J. Garrett 219 (1994) 409
Holden, J.M., see Y. Wang 211 (1993) 341; 217 (1994) 413
Holden, J.M., P. Zhou, X.-X. Bi, P.C. Eklund, S. Bandow, R.A. Jishi, K. Das Chowdhury, G. Dresselhaus and M.S. Dresselhaus, Raman scattering from nanoscale carbons generated in a cobalt-catalyzed carbon plasma 220 (1994) 186
Holme, T.A. and T.N. Truong, A test of density functional theory for dative bonding systems 215 (1993) 53
Holmes, A.B., see I.D.W. Samuel 213 (1993) 472
Holmes, A.B., see M. Fahlman 214 (1993) 327
Holmes, J.L., F.P. Lossing and P.M. Mayer, The effects of methyl substitution on the structure and thermochemistry of the cyanomethyl radical and cation 212 (1993) 134
Holovko, M.F., see Yu.V. Kalyuzhnyi 215 (1993) 1
Holtgrave, J., K. Riehl, D. Abner and P.D. Haaland, Ion chemistry in tetraethylorthosilicate $(C_2H_5O)_4Si$ 215 (1993) 548
Holtom, G.R., see R. Knochenmuss 215 (1993) 188
Hömmerich, U., see H. Eilers 212 (1993) 109
Hömmerich, U., H. Eilers, W.M. Yen and H.R. Verdún, The optical center $M_nO_4^{3-}$ in Y_2SiO_5:Mn, X (X=Al, Ca) 213 (1993) 163
Honigmann, M., see Y. Li 212 (1993) 185
Hönle, W., see K. Kamarás 214 (1993) 338
Honma, C., see T. Nakayama 213 (1993) 581
Hoppe, R., see G. Blasse 215 (1993) 363
Horani, M., see S. Douin 216 (1993) 215
Horiai, K., see H. Uehara 213 (1993) 101; 214 (1993) 527; 215 (1993) 505
Hormes, J., see S. Grimme 213 (1993) 32
Horoyski, P.J. and M.L.W. Thewalt, C_{70} vibrational frequencies obtained from singlet oxygen photoluminescence 217 (1994) 409
Horsewill, A.J., see S. Clough 211 (1993) 637
Hoshino, K., T. Naganuma, K. Watanabe, A. Nakajima and K. Kaya, Ionization potentials of gold–sodium (Au_nNa_m) bimetallic clusters 211 (1993) 571
Hoshino, K., see A. Nakajima 214 (1993) 22
Hotokka, M., see O.-P. Sairanen 215 (1993) 353
Houde, D., see T.-H. Tran-Thi 213 (1993) 139
Howard, S.T. and K. Woźniak, The effect of electron correlation on the structure and properties of the benzenium ion 212 (1993) 1
Howdle, S.M. and V.N. Bagratashvili, The effects of fluid density on the rotational Raman spectrum of hydrogen dissolved in supercritical carbon dioxide 214 (1993) 215
Hrbek, J., see J.A. Rodriguez 220 (1994) 486
Hrušák, J., see A. Fiedler 211 (1993) 242
Hsieh, T.-C., see T.-C. Chang 213 (1993) 564
Hsue, C.-S., see C.-C. Chen 217 (1994) 486
Huang, K.L., see B. Fain 216 (1993) 551
Huang, R., J. Wu, M.-X. Gong, A. Saury and E. Carrasquillo M., Direct observation of vibrational relaxation in highly excited HCN 216 (1993) 108
Huang, R., J. Wu, M.-X. Gong, A. Saury and E. Carrasquillo M., Vibrational state-to-state resolution in the collisional relaxation of a highly vibrationally excited polyatomic: HCN 216 (1993) 115

Huang, Y. and S.-I Chu, Study of the photoabsorption spectrum of diamagnetic Rydberg atoms without the need of using full eigenvectors 211 (1993) 601
Huang, Y., W. Zhu, D.J. Kouri and D.K. Hoffman, A general time-to-energy transform of wavepackets. Time-independent wavepacket-Schrödinger and wavepacket-Lippmann–Schwinger equation (Chem. Phys. Letters 206 (1993) 96). Erratum 213 (1993) 209
Huang, Y., W. Zhu, D.J. Kouri and D.K. Hoffman, Analytic continuation of the polynomial representation of the full, interacting time-independent Green function 214 (1993) 451
Huang, Y., see W. Zhu 217 (1994) 73
Huang, Y., see D.J. Kouri 220 (1994) 312
Huber, J.R., see M.-A. Thelen 213 (1993) 275
Huber, J.R., see G. Baum 213 (1993) 427
Huber, J.R., see P. Felder 215 (1993) 221
Huber, J.R., see G.P. Morley 219 (1994) 195
Hubrich, M., G.G. Maresch and H.W. Spiess, Pulsed electron nuclear double resonance study of molecular motions of radicals in a high-strength liquid-crystalline polymer 218 (1994) 81
Huché, M., see M. Lequan 213 (1993) 71
Hudson, E., see G. Remmers 214 (1993) 241
Huffman, D.R., see L. Nemes 218 (1994) 295
Huisken, F., see M. Ehbrecht 214 (1993) 34
Hulett Jr. , L.D., D.L. Donohue, J. Xu, T.A. Lewis, S.A. McLuckey and G.L. Glish, Mass spectrometry studies of the ionization of organic molecules by low-energy positons 216 (1993) 236
Hunter, C.N., see H. van der Laan 212 (1993) 569
Hurley, M.D., see T.J. Wallington 211 (1993) 41; 213 (1993) 442; 218 (1994) 34
Hurwitz, Y., Y. Rudich and R. Naaman, Reactant rotational energy effect on energy distribution in products. The role of the electronic angular momentum 215 (1993) 674
Hüttermann, J., see S.A. Dikanov 212 (1993) 493
Huuang, J.-S., see W.-D. Cheng 216 (1993) 353
Huzinaga, S. and M. Klobukowski, Well-tempered Gaussian basis sets for the calculation of matrix Hartree–Fock wavefunctions 212 (1993) 260
Hvelplund, P., see L.H. Andersen 217 (1994) 204
Hvidt, A., see P. Westh 217 (1994) 245

Ibuki, K., see T. Nakayama 215 (1993) 622; 220 (1994) 219
Igarashi, M., see Y. Nakamura 217 (1994) 387
I'Haya, Y.J. and S. Kanosue, Solvent dependence of excited molecule-free radical interactions studied by means of time-resolved electron spin resonance 216 (1993) 231
I'Haya, Y.J., see K. Kobayashi 219 (1994) 53
Iijima, T., Anharmonicity of the OH...O hydrogen bond in liquid water 217 (1994) 503
Ikeda, H., see H. Umemoto 214 (1993) 271
Ikeda, R., see N. Kimura 220 (1994) 40
Ikemoto, I., see K. Kikuchi 216 (1993) 67
Ikeura, H., K. Tanaka, T. Sekiguchi and K. Obi, Observation of neutral products of a soft X-ray stimulated etching reaction in the SF_6/a-SiO_2 absorption system 217 (1994) 131
Ikeyama, T. and T. Azumi, Triplet spin-sublevel selectivity of the S_1–T_1 intersystem crossing in trans-stilbene 212 (1993) 551
Illas, F., see C. Sousa 215 (1993) 97
Illas, F., see J. Rubio 217 (1994) 283
Imamura, A., see Y. Kohno 214 (1993) 603
Inaba, R., K. Tominaga, M. Tasumi, K.A. Nelson and K. Yoshihara, Observation of homogeneous vibrational dephasing in benzonitrile by ultrafast Raman echoes 211 (1993) 183
Infante, G., see G. Polzonetti 214 (1993) 333
Iogansen, A.A., O.M. Sarkisov, E.V. Zimont, J.A. Seetula, R.S. Timonen and S. Cheskis, Formation of vibrationally excited OH radicals in the $O(^1D) + H_2S$ reaction 212 (1993) 604
Ionov, P.I., see H.F. Davis 215 (1993) 214
Ionov, S.I., see H.F. Davis 215 (1993) 214
Irngartinger, T., see F. Güttler 217 (1994) 393
Irving, K., see O.N. Ventura 217 (1994) 436
Ishida, T., A classical cross-section calculation for Penning ionization with multi-exit channels. N_2–$He^*(2\,^3S) \rightarrow N_2^+(^2\Sigma_g, ^2\Pi_u, ^2\Sigma_u) + He + e^-$ 211 (1993) 1
Ishii, J., T. Matsui, K. Tsukiyama and K. Uehara, Observation of the $A\,^2\Sigma^+ \leftarrow X\,^2\Pi_{3/2}$ transition of nitric oxide with two-photon degenerate four-wave mixing 220 (1994) 29
Ishikawa, M. and Y. Maruyama, Femtosecond spectral hole-burning of crystal violet in methanol. New evidence for ground state conformers 219 (1994) 416
Ishikawa, Y., see X. Gu 211 (1993) 65
Ishikawa, Y., Comment on "Segmented contractions of relativistic Gaussian basis sets" 212 (1993) 547
Ishikawa, Y., Ab initio study of the structure and ionization potential of aluminum–sodium bimetallic cluster, Al_2Na 213 (1993) 527
Ishikawa, Y., see V. Keshari 218 (1994) 406
Islampour, R., see M. Hayashi 213 (1993) 465
Ito, A., T. Morikawa and T. Takahashi, Photo-induced polymerization and oxidation of C_{60} observed by photoelectron spectroscopy 211 (1993) 333
Ito, M., see M. Mimuro 213 (1993) 576
Ito, S., see H. Sekiya 215 (1993) 499
Ito, Y., see K. Yamasaki 215 (1993) 483
Itoh, I., see M. Yagi 211 (1993) 179
Itoh, M., see H. Mukaihata 211 (1993) 140
Itoh, M., see R. Takasu 217 (1994) 478
Ivanov, A.I. and V.A. Mikhaylova, The effect of a magnetic field on outer-sphere electron transfer 212 (1993) 697
Iwata, S., see M. Hiyama 211 (1993) 319

Jackson, W.M., see M. Gong 217 (1994) 210
Jackson, W.M., see X. Song 217 (1994) 216
Jackson, W.M., see V.R. Morris 220 (1994) 448
Jacobs, A., H.-R. Volpp and J. Wolfrum, Reaction dynamics, OH energy partitioning, and OH product angular momentum alignment studies: $H+H_2O \rightarrow OH+H_2$ versus $H+CO_2 \rightarrow OH+CO$ 218 (1994) 51
Jacobs, W.P.J.H., see M.J.P. Brugmans 217 (1994) 117
Jacobsen, S.M., see H. Eilers 212 (1993) 109
Jacques, P., see E. Vauthey 215 (1993) 264
Jaeger, C., see M.E. Smith 219 (1994) 75
Jäger, W., see S. Schneider 219 (1994) 433
Jahn, L.G., see J.P. Culver 214 (1993) 431
Jakobi, M., see J. Fulara 211 (1993) 227
Jamali, J.B., see K. Mukai 214 (1993) 559
James, A.M., P. Kowalczyk and B. Simard, First observation of the VNb molecule 216 (1993) 512
James, G.K., see I. Kanik 211 (1993) 523
Janicke, M., see R.G. Larsen 214 (1993) 220
Jansen, G., B.A. Hess and P.E.S. Wormer, Theoretical investigation of the rovibrational fine-structure spectrum of Ar–NH in its electronic ground state 214 (1993) 103
Jansen, G., see J.G. Ángyán 219 (1994) 267
Janssen, M.H.M., M. Dantus, H. Guo and A.H. Zewail, Femtosecond reaction dynamics of Rydberg states. Methyl iodide 214 (1993) 281
Janszky, J., P. Adam, An.V. Vinogradov and T. Kobayashi, Vibrational state shaping for selective laser chemistry 213 (1993) 368
Jaque, F., see U. Caldiño G. 213 (1993) 84
Jasinski, J.M., Formation of gas-phase silyl radicals in the atomic hydrogen etching of silicon 211 (1993) 564
Jasra, R.V., N.V. Choudary, K.V. Rao, G.C. Pandey and S.G.T. Bhat, Far-IR spectroscopic studies on zeolite NaCaA 211 (1993) 214
Jaszunski, M., T. Helgaker, K. Ruud, K.L. Bak and P. Jørgensen, MCSCF calculations of nitrogen NMR shielding constants using London atomic orbitals 220 (1994) 154
Jayannavar, A.M., see G.V. Raviprasad 220 (1994) 353
Jayatilaka, D., Analytic SCF third and fourth derivatives with model potentials 212 (1993) 18
Jeevarajan, A.S., L.D. Kispert and X. Wu, Spectroelectrochemistry of carotenoids in solution 219 (1994) 427
Jemmis, E.D., see G. Subramanian 217 (1994) 296
Jena, P., see S.N. Khanna 218 (1994) 383; 219 (1994) 479
Jenkin, M.E., see T.J. Wallington 211 (1993) 41
Jensen, J.O., see P.N. Krishnan 217 (1994) 311
Jensen, V.R. and P.E.M. Siegbahn, The Ziegler–Natta olefin insertion reaction for cationic metals 212 (1993) 353
Jeung, G.-H., see T. Leininger 220 (1994) 345
Jiang, B., see W. Sun 218 (1994) 515
Jiao, J., see S. Seraphin 217 (1994) 191
Jiménez-Mier, J., see S.J. Schaphorst 213 (1993) 315
Jin, S., see J.D. Head 212 (1993) 32
Jishi, R.A., see J.M. Holden 220 (1994) 186
Joachim, C., see C. Chavy 214 (1993) 569; 219 (1994) 502
Jochims, H.W., see E. Rühl 211 (1993) 403

Johnson, A.E., S. Kumazaki and K. Yoshihara, Pump–probe spectroscopy and exciton dynamics of J aggregates at high pump intensities 211 (1993) 511
Johnson, B.G., see K. Raghavachari 214 (1993) 357; 220 (1994) 385
Johnson, B.G. and M.J. Frisch, Analytic second derivatives of the gradient-corrected density functional energy. Effect of quadrature weight derivatives 216 (1993) 133
Johnson, B.G., see P.M.W. Gill 217 (1994) 65
Johnson, B.G., J.A. Pople, P.M.W. Gill and D.J. Fox, Reply to Comment on "Computing molecular electrostatic potentials with the PRISM algorithm" 218 (1994) 595
Johnson, B.G., P.M.W. Gill and J.A. Pople, A rotationally invariant procedure for density functional calculations 220 (1994) 377
Johnson, K.H., see T.S. Smit 212 (1993) 525
Johnson, M.A., see M.A. Buntine 216 (1993) 471
Johnson, M.R., see S. Clough 211 (1993) 637
Johnson, P.D., see M. Neeb 212 (1993) 205
Johnson, R.D., see C.-H. Park 213 (1993) 196
Jonas, J., see S. Xu 218 (1994) 329
Jones, A.C., M.J. Dale, G.A. Keenan and P.R.R. Langridge-Smith, Photoionisation and photodissociation of laser-vaporised metallotetraphenylporphyrins 219 (1994) 174
Jones, J.D., see D.A. Butler 217 (1994) 423
Jones, R.B., S.L. Allman, K. Tang, W.R. Garrett and C.H. Chen, Neutralization of negatively charged oligonucleotides 212 (1993) 451
Jongma, R.T., see G. Meijer 217 (1994) 112
Jonker, M., see G. van den Hoek 215 (1993) 461
Jordan, K.D., see C.J. Tsai 213 (1993) 181
Jordan, K.D., see K. Kim 218 (1994) 261
Jørgensen, P., see R. Kobayashi 211 (1993) 94; 215 (1993) 576; 219 (1994) 30
Jørgensen, P., see Y. Luo 213 (1993) 356
Jørgensen, P., see M. Jaszunski 220 (1994) 154
Joslin, C.G., J. Yang, C.G. Gray, S. Goldman and J.D. Poll, Infrared rotation and vibration–rotation bands of endohedral fullerene complexes. $K^+@C_{60}$ 211 (1993) 587
Joslin, C.G., C.G. Gray, J.D. Goddard, S. Goldman, J. Yang and J.D. Poll, Infrared rotation and vibration–rotation bands of endohedral fullerene complexes. $He@C_{60}$ 213 (1993) 377
Joslin, C.G., C.G. Gray, S. Goldman, J. Yang and J.D. Poll, Raman spectra of endohedral fullerenes. $Li^+@C_{60}$ 215 (1993) 144
Joutsensaari, J., see A.S. Gurav 218 (1994) 304
Jouvet, C., see S. Martrenchard-Barra 215 (1993) 291
Jovanic, B.R., Lj.D. Zekovic and B. Radenkovic, Theoretical calculations of the pressure-induced shift of a photoacoustic phase signal in alexandrite ($BeAl_2O_4:Cr^{3+}$) 216 (1993) 47
Judeinstein, P., P.W. Oliveira, H. Krug and H. Schmidt, Dynamics of the sol–gel transition in organic–inorganic nanocomposites 220 (1994) 35
Jug, K., see T. Kar 214 (1993) 615
Jullien, S., J. Lemaire, S. Fenistein, M. Heninger, G. Mauclaire and R. Marx, Radiative lifetimes of Xe^+ and Kr^+ in their $^2P_{1/2}$ spin–orbit states 212 (1993) 340
Jungwirth, P. and R. Zahradník, Is the water-induced potential of mean torsion of *n*-butane transferable to longer *n*-alkanes? 212 (1993) 211
Jungwirth, P. and R. Zahradník, The entropy driven hydrophobic effect as a function of solute–solvent interactions. A molecular dynamics study 217 (1994) 319

Juvan, K.A., see J.L. Cheung 213 (1993) 309
Jux, N., see A. Berman 211 (1993) 549

Kachanov, A.A., see A. Charvát 214 (1993) 495
Kaindl, G., see G. Remmers 214 (1993) 241
Kais, S., see D.J. Lacks 218 (1994) 229
Kajzar, F., C. Taliani, R. Danieli, S. Rossini and R. Zamboni, Wave-dispersed third-order nonlinear optical properties of C_{60} thin films 217 (1994) 418
Kalcher, J. and A.F. Sax, Stabilities and stationary points for singlet and triplet states of the Si_2H^- anion 215 (1993) 601
Kalcher, J., see M.C. Ernst 216 (1993) 189
Kalinowski, J., see G. Giro 211 (1993) 580
Kalontarov, L.I., Kinetic regularities for laser-induced thermal reactions of polymers 217 (1994) 222
Kalyuzhnyi, Yu.V., I.A. Protsykevytch and M.F. Holovko, Solution of the associative Percus–Yevick approximation for the *n*-component mixture of dimerizing hard spheres 215 (1993) 1
Kalyuzhnyi, Yu.V. and V. Vlachy, Integral equation theory for highly asymmetric electrolyte solutions 215 (1993) 518
Kamalov, V.F., I.A. Struganova and K. Yoshihara, Time-resolved emission spectra of the BIC J-aggregate at low temperature 213 (1993) 559
Kamalov, V.F., I.A. Struganova, T. Tani and K. Yoshihara, Temperature dependence of superradiant emission of BIC J-aggregates 220 (1994) 257
Kamarás, K., L. Akselrod, S. Roth, A. Mittelbach, W. Hönle and H.G. von Schnering, The orientational phase transition in C_{60} films followed by infrared spectroscopy 214 (1993) 338
Kaminskii, A.A., see U. Caldiño G. 213 (1993) 84
Kandori, H., K. Yoshihara, H. Tomioka, H. Sasabe and Y. Shichida, Comparative study of primary photochemical events of two retinal proteins, bacteriorhodopsin and halorhodopsin, by use of subpicosecond time-resolved spectroscopy 211 (1993) 385
Kandori, H. and H. Sasabe, Excited-state dynamics of a protonated Schiff base of all-trans retinal in methanol probed by femtosecond fluorescence measurement 216 (1993) 126
Kanematsu, Y., see J.S. Ahn 215 (1993) 336
Kanik, I., J.M. Ajello and G.K. James, Extreme ultraviolet emission spectrum of CO_2 induced by electron impact at 200 eV 211 (1993) 523
Kanosue, S., see Y.J. I'Haya 216 (1993) 231
Kaplan, I.G., see R. Santamaria 218 (1994) 395
Kar, T. and K. Jug, The remarkable stability of the $LiBH_2$ and $HBeBH_2$ dimers. B=B double bond or multi-center bonds? 214 (1993) 615
Kar, T., P.K. Nandi and A.B. Sannigrahi, Bonding in beryllium carbonyls 220 (1994) 133
Karawajczyk, A., see P. Erman 215 (1993) 173
Karna, S.P., A "direct" time-dependent coupled perturbed Hartree–Fock–Roothaan approach to calculate molecular (hyper)polarizabilities 214 (1993) 186
Karthäuser, J., see I.R. Sims 211 (1993) 461
Karwasz, G., R.S. Brusa, A. Gasparoli and A. Zecca, Total cross-section measurements for e^-–CO scattering: 80–4000 eV 211 (1993) 529
Kasemo, B., see M. Rinnemo 211 (1993) 60
Kasuya, A., see Y. Saito 212 (1993) 379
Katayama, D.H., see J.M. Thomas 214 (1993) 250
Kato, S., see S. Ten-no 214 (1993) 391
Katoh, T., see M. Mimuro 213 (1993) 576
Kaufman, J.J., see S. Roszak 215 (1993) 427
Kauppi, E., see J. Nieminen 217 (1994) 31

Kauppinen, E.I., see A.S. Gurav 218 (1994) 304
Kawai, A., Y. Kobori and K. Obi, Time-resolved ESR spectra of the α-hydroxybenzyl–amine complex 215 (1993) 203
Kawai, M., see J. Yoshinobu 211 (1993) 48
Kawai, M., see N. Takagi 215 (1993) 120
Kawamori, A., see S.A. Dzuba 214 (1993) 621
Kawasaki, M., see M. Ohashi 220 (1994) 7
Kaya, K., see K. Hoshino 211 (1993) 571
Kaya, K., see A. Nakajima 214 (1993) 22
Kedzierski, W., J.B. Atkinson and L. Krause, Laser-induced fluorescence from the $^3\Pi_u(4\ ^3P, 4\ ^3P)$ state of Zn_2 215 (1993) 185
Kedzierski, W., J. Supronowicz, A. Czajkowski, M.J. Hinek, J.B. Atkinson and L. Krause, The rotationally resolved $G0_u^+ \leftarrow A0_g^+$ electronic spectrum of the $(^{202}Hg)_2$ excimer 218 (1994) 314
Keeling, L.A., L. Chen, C.M. Greenlief, A. Mahajan and D. Bonser, Direct evidence for β-hydride elimination on Si(100) 217 (1994) 136
Keenan, G.A., see A.C. Jones 219 (1994) 174
Keita, B., L. Nadjo, R. Céolin, V. Agafonov, D. André, H. Szwarc, J. Dugué, C. Fabre, A. Rassat and P.-Y. Sizaret, Scanning tunneling microscopy study of the surface of C_{60} decagonal crystals grown from *n*-hexane 215 (1993) 125
Kelly, C., H.W. Sidebottom, J. Treacy and O.J. Nielsen, Reactions of CF_3O radicals with selected alkenes and aromatics under atmospheric conditions 218 (1994) 29
Kelly, H.M., see P.W. Fowler 212 (1993) 659; 216 (1993) 200
Kelner, V., see E. Sominska 213 (1993) 117
Kerim, A., see H. Uehara 213 (1993) 101
Keshari, V. and Y. Ishikawa, Ab initio Monte Carlo simulated annealing method 218 (1994) 406
Keshavamurthy, S. and W.H. Miller, Semi-classical correction for quantum-mechanical scattering 218 (1994) 189
Khan, A., Theoretical studies of the clathrate structures of $(H_2O)_{20}$, $H^+(H_2O)_{20}$ and $H^+(H_2O)_{21}$ 217 (1994) 443
Khanna, S.N. and P. Jena, Reactivity of hydrogen with open and closed shell clusters 218 (1994) 383
Khanna, S.N. and P. Jena, Designing ionic solids from metallic clusters 219 (1994) 479
Kharlamov, A.A., L.A. Chernozatonskii and A.A. Dityat'ev, Two states of C_{60} film at the air/water interface 219 (1994) 457
Khmelenko, V.V., see E.B. Gordon 217 (1994) 605
Khmelinskii, I.V., see S.A. Nizkorodov 215 (1993) 662
Kiefer, W., see C. Engert 218 (1994) 87
Kikuchi, K., S. Suzuki, Y. Nakao, N. Nakahara, T. Wakabayashi, H. Shiromaru, K. Saito, I. Ikemoto and Y. Achiba, Isolation and characterization of the metallofullerene LaC_{82} 216 (1993) 67
Kilcoyne, A.L.D., see M. Neeb 212 (1993) 205
Kim, B. and K. Yoshihara, $^3\Delta$–$^1\Sigma^+$ transition of RbCs observed in a very cold molecular beam 212 (1993) 271
Kim, D., see E. Shin 218 (1994) 107
Kim, D.Y., see D.A. Baugh 219 (1994) 207
Kim, J., see B.J. Mhin 216 (1993) 305
Kim, J., see K.S. Kim 216 (1993) 309
Kim, J., B.J. Mhin, S.J. Lee and K.S. Kim, Entropy-driven structures of the water octamer 219 (1994) 243
Kim, K. and K.D. Jordan, Theoretical calculation of the height of the barrier for OH rotation in phenol 218 (1994) 261

Kim, K.S., see B.J. Mhin 216 (1993) 305
Kim, K.S., S. Lee, B.J. Mhin, S.J. Cho and J. Kim, Structures and energetics of $Zn(NH_3)_n^{2+}$ ($n=4$–6). Coordination number of Zn^{2+} by ammine 216 (1993) 309
Kim, K.S., see J. Kim 219 (1994) 243
Kim, S.K., see E. Shin 218 (1994) 107
Kim, Y.J., see S. Xu 218 (1994) 329
Kimachi, S., see H. Miki 218 (1994) 563
Kimura, N., H. Ohki, R. Ikeda and M. Yamashita, Valence structure of one-dimensional halogen bridged –Pt–Pt–X–Pt–Pt–X– type complexes studied by ^{31}P solid NMR 220 (1994) 40
King-Smith, R.D., see F. Liu 215 (1993) 401
Kinuchi, K., see F. Negri 211 (1993) 353
Kishi, R., see A. Nakajima 214 (1993) 22
Kishinevsky, H.M., see J.J. Borrás-Almenar 217 (1994) 525
Kiskinova, M., see D. Alfè 211 (1993) 220
Kispert, L.D., see A.S. Jeevarajan 219 (1994) 427
Kiyobayashi, T., see Y. Nagano 217 (1994) 186
Klafter, J., see G. Zumofen 219 (1994) 303
Kleiber, P.D., see L.N. Ding 212 (1993) 499
Klein, D.J., see D. Babić 211 (1993) 235
Klein, D.J., Graphitic polymer strips with edge states 217 (1994) 261
Klein, D.J., see A.T. Balaban 217 (1994) 266
Klein, M.L., see M. Ferrario 213 (1993) 537
Klein, U.K.A., see K.A. Al-Hassan 212 (1993) 581
Klein, U.K.A., J. Mastromarino, Z.H. Yamani and A. Suwaiyan, Fluorescence demodulation spectroscopy. A new method of determining fluorescence decays using two beating ring dye lasers 217 (1994) 80
Klein, U.K.A., J. Mastromarino and A. Suwaiyan, Rotational level lifetimes and self-quenching of $^{127}I_2$ by fluorescence demodulation spectroscopy 217 (1994) 86
Kleindienst, H., see A. Lüchow 216 (1993) 359
Kleindienst, H., A. Lüchow and H.-P. Merckens, Accurate upper and lower bounds for some excited S states of the He atom 218 (1994) 441
Kleinermanns, K., see J. Schlütter 213 (1993) 262
Kleinermanns, K., see M. Schmitt 218 (1994) 246
Klemm, R.B., see P.S. Monks 211 (1993) 416
Kleyn, A.W., see A.E. Wiskerke 216 (1993) 93
Kleyn, A.W., see M.J.P. Brugmans 217 (1994) 117
Klink, C., see M. Foss 215 (1993) 535
Klinowski, J., see B. Herreros 220 (1994) 478
Klippenstein, S.J., The evaluation of $N_E(R)$ within a variably defined reaction coordinate framework 214 (1993) 418
Klobukowski, M., see S. Huzinaga 212 (1993) 260
Klobukowski, M., Comparison of generator formulas for exponential parameters of Gaussian basis sets 214 (1993) 166
Klos, H., see A. Skiebe 220 (1994) 138
Kneipp, H., K. Kneipp and F. Seifert, Surface-enhanced hyper-Raman scattering (SEHRS) and surface-enhanced Raman scattering (SERS) by means of mode-locked Ti:sapphire laser excitation 212 (1993) 374

Kneipp, K., see H. Kneipp 212 (1993) 374
Knight, A.E.W., see J.S. Francisco 214 (1993) 77
Knochenmuss, R., G.R. Holtom and D. Ray, Proton transfer reaction rates as a probe of size-dependent properties of large water clusters 215 (1993) 188
Knoll, W., see Z. Sekkat 220 (1994) 497
Knuth, E.L. and H.-G. Rubahn, Cross sections for rotational relaxation in alkali dimer molecular beams 213 (1993) 1
Knuts, S., see Y. Luo 213 (1993) 356
Kobayashi, K., see S. Nagase 214 (1993) 57
Kobayashi, K., T. Sano and Y.J. I'Haya, Quasi-particle energy band structure and core-electron transition energy calculation for two-dimensional hexagonal boron nitride 219 (1994) 53
Kobayashi, R., H. Koch, P. Jørgensen and T.J. Lee, Comparison of coupled-cluster and Brueckner coupled-cluster calculations of molecular properties 211 (1993) 94
Kobayashi, R., O. Bludský, H. Koch and P. Jørgensen, Quartic coupled cluster force fields for the diazene isomers 215 (1993) 576
Kobayashi, R., H. Koch and P. Jørgensen, Calculation of frequency-dependent polarizabilities using coupled-cluster response theory 219 (1994) 30
Kobayashi, T., see J. Janszky 213 (1993) 368
Kobayashi, T., see K. Minoshima 218 (1994) 67
Kobayashi, T., see K. Misawa 220 (1994) 251
Kobe, K., H. Kühling, S. Rutz, E. Schreiber, J.P. Wolf, L. Wöste, M. Broyer and Ph. Dugourd, Time-resolved observation of molecular pseudorotation in Na_3 213 (1993) 554
Kobori, Y., see A. Kawai 215 (1993) 203
Koch, H., see R. Kobayashi 211 (1993) 94; 215 (1993) 576; 219 (1994) 30
Koch, H. and E. Dalgaard, Linear superposition of optimized non-orthogonal Slater determinants for singlet states 212 (1993) 193
Koch, R., B. Burg, K. Schmidt, K.H. Rieder, E. Schwarz and K. Christmann, Oxygen adsorption on Co($10\bar{1}0$). The structure of p(2×1)2O 220 (1994) 172
Koch, W., see A. Fiedler 211 (1993) 242
Koch, W., see W.P. Kraemer 212 (1993) 631
Kochanski, G.P., see R.C. Haddon 218 (1994) 100
Kodas, T.T., see A.S. Gurav 218 (1994) 304
Kodera, Y., see S.A. Dzuba 214 (1993) 621
Koga, Y., see P. Westh 217 (1994) 245
Kohanoff, J., see G. Onida 219 (1994) 1
Kohno, J., see F. Mafuné 218 (1994) 7
Kohno, Y., K. Maekawa, T. Tsuchioka, T. Hashizume and A. Imamura, A molecular orbital study on the effects of electron correlation on the unique N–N bond in nitramines 214 (1993) 603
Koizumi, H., Photoionization quantum yield for liquid squalane and squalene estimated from photoelectron emission yield 219 (1994) 137
Kolasinski, K.W., F. Cemic and E. Hasselbrink, O_2/Pd(111). Clarification of the correspondence between thermal desorption features and chemisorption states 219 (1994) 113
Kolb, D., see T. Baştuğ 211 (1993) 119
Kolbuszewski, M. and J.S. Wright, Thermodynamically stable diatomic dications: MgN^{2+}, MgO^{2+}, MgF^{2+} and MgNe 218 (1994) 338
Kolesnick, R.E., see G.D. Billing 215 (1993) 571
Kolibiar, M., M. Foltin and T.D. Märk, Molecular dynamics simulation of Xe^+ ion collisions with Ar_{29} and Ne_{29} clusters 219 (1994) 252

Komaromi, I. and J.M.J. Tronchet, The geometry of the H_2NO radical: do the quantum mechanical results converge? 215 (1993) 444
Kominami, K., see K. Sakoda 215 (1993) 488; 216 (1993) 270
Kompa, K.L., see K.L. Bintz 215 (1993) 455
Komura, A., see M. Yagi 211 (1993) 179
Kondepudi, D.K. and C. Sabanayagam, Secondary nucleation that leads to chiral symmetry breaking in stirred crystallization 217 (1994) 364
Kondow, T., see T. Tsukuda 218 (1994) 1
Kondow, T., see F. Mafuné 218 (1994) 7, 234
Kong, J., L.A. Eriksson and R.J. Boyd, A density functional theory study of the hyperfine structures of the atoms B to O and the species NH_2 and NH_3^+ 217 (1994) 24
Konishi, Y., see A. Nakajima 214 (1993) 22
Konno, T., see H. Uehara 213 (1993) 101; 214 (1993) 527; 215 (1993) 505
Kono, H., Extraction of eigenstates from an optically prepared state by a time-dependent quantum-mechanical method. Toward simulation of "intermediate case" radiationless transitions 214 (1993) 137
Kono, T., see T. Gejo 218 (1994) 343
Konrat, R., G. Zieger and H. Sterk, Directed coherence transfer in nuclear magnetic resonance. Two-dimensional in-phase multiplets in selective correlation spectroscopy 212 (1993) 78
Konvička, K., see J. Vacek 220 (1994) 85
Koperski, J., J.B. Atkinson and L. Krause, The $0_u^+(6\ ^3P_1) \leftarrow X0_g^+$ spectrum of Hg_2 excited in a supersonic jet 219 (1994) 161
Koppe, S., T. Laurent, P.D. Naik, H.-R. Volpp, J. Wolfrum, T. Arusi-Parpar, I. Bar and S. Rosenwaks, Absolute rate constants and reactive cross sections for the reactions of $O(^1D)$ with molecular hydrogen and deuterium 214 (1993) 546
Kornyshev, A.A. and K.M. Robinson, Interfacial electronic profile from X-ray reflectivity 219 (1994) 132
Koroteev, N.I., see V.D. Vachev 215 (1993) 306
Korppi-Tommola, J.E.I., see E. Laitinen 218 (1994) 73
Koski, W.S., see S. Roszak 215 (1993) 427
Kossanyi, J., see S. Bachir 213 (1993) 54
Kotschubei, S.A., see S.A. Nizkorodov 215 (1993) 662
Koubi, L., M. Blain, E. Cohen de Lara and J.-M. Leclercq, Vibrational frequency shifts of diatomic molecules in interaction with a Na^+ cation by ab initio calculations. Comparison with experiment on H_2 and N_2 adsorbed in NaA zeolite 217 (1994) 544
Kouri, D.J., see Y. Huang 213 (1993) 209; 214 (1993) 451
Kouri, D.J., see W. Zhu 217 (1994) 73
Kouri, D.J., W. Zhu, Y. Huang and D.K. Hoffman, Analytical evaluation of the energy derivative of the *S* matrix in the time-independent wavepacket approach to quantum scattering 220 (1994) 312
Kouyaté, D., see S. Bachir 213 (1993) 54
Kowalczyk, P., see A.M. James 216 (1993) 512
Kozankiewicz, B., Migration of CT triplet excitons in TCNB-biphenyl and TCNB-HMB crystals 217 (1994) 91
Kraabel, B., C.H. Lee, D. McBranch, D. Moses, N.S. Sariciftci and A.J. Heeger, Ultrafast photoinduced electron transfer in conducting polymer–buckminsterfullerene composites 213 (1993) 389
Kraemer, W.P. and W. Koch, A CASSCF-CI study of the ground and low-lying excited electronic states of $C_2H_2^+$ 212 (1993) 631

Kraka, E. and D. Cremer, Ortho-, meta-, and para-benzyne. A comparative CCSD(T) investigation 216 (1993) 333
Kraka, E. and D. Cremer, Ortho-, meta-, and para-benzyne. A comparative CCSD (T) investigation (Chem. Phys. Letters 216 (1993) 333). Addendum 219 (1994) 160
Krämer, U., see K.L. Walther 212 (1993) 96
Krause, H. and H.J. Neusser, The van der Waals modes of the (benzene–Ar)$^+$ complex studied by mass selective pulsed field threshold ionization 213 (1993) 603
Krause, L., see J. Supronowicz 213 (1993) 282; 218 (1994) 240
Krause, L., see W. Kedzierski 215 (1993) 185; 218 (1994) 314
Krause, L., see J. Koperski 219 (1994) 161
Krause, M.O., see S.J. Schaphorst 213 (1993) 315
Krauss, M., see P.S. Monks 211 (1993) 416
Krausz, E., see H. Riesen 212 (1993) 347; 217 (1994) 613; 218 (1994) 579
Kreisle, D., see K. Athanassenas 213 (1993) 105
Krishnamurthy, M. and D. Mathur, Collision-induced dissociation of oriented CO^+ ions. Probing potential energy curves by ion collision spectrometry 216 (1993) 203
Krishnan, P.N., J.O. Jensen and L.A. Burke, Theoretical study of water clusters. II. Hexamer 217 (1994) 311
Kronseder, C., see C. Berg 216 (1993) 465
Kroto, H.W. and D.R.M. Walton, Stable derivatives of small fullerenes 214 (1993) 353
Krug, H., see P. Judeinstein 220 (1994) 35
Krüger, S. and N. Rösch, Embedding effects on core level shifts of surface cluster models 216 (1993) 435
Krzysztofowicz, A.M. and C. Szmytkowski, Electron scattering from methyl bromide. Absolute total cross section measurements 219 (1994) 86
Ku, J.K., see K. Lee 216 (1993) 483
Kubach, C., see G. Nguyen Vien 215 (1993) 35
Kuczkowski, R.L., see S.E. Forest 218 (1994) 349
Kudriavtsev, N.N., D.P. Shamshev and A.M. Sukhov, Chemiluminescence observations in the potential exchange NF–IF laser system 214 (1993) 513
Kuga, T., see J. Takeda 220 (1994) 443
Kühling, H., see K. Kobe 213 (1993) 554
Kukk, P., see A. Freiberg 214 (1993) 10
Kukolich, S.G. and S.M. Sickafoose, The microwave spectrum and Mn–H bond length for $HMn(CO)_5$ 215 (1993) 168
Kumar, G.R., C.P. Safvan, F.A. Rajgara and D. Mathur, Intense laser field ionisation of CS_2 at 532 nm. Does dissociation precede ionisation? 217 (1994) 626
Kumazaki, S., see A.E. Johnson 211 (1993) 511
Kunst, M., see C.M. Haffer 211 (1993) 203
Kuo, S.C., see P.S. Monks 211 (1993) 416
Kuppermann, A. and Y.-S.M. Wu, The geometric phase effect shows up in chemical reactions (Chem. Phys. Letters 205 (1993) 577). Erratum 213 (1993) 636
Kurita, S., see J. Takeda 220 (1994) 443
Kurita, Y., see J. Takeda 220 (1994) 443
Kurreck, H., see S.D. Chemerisov 218 (1994) 353
Kusalik, P.G., see I.M. Svishchev 215 (1993) 596
Kushch, N.D., I. Majchrzak, W. Ciesielski and A. Graja, Preparation and spectral properties of $C_{60}S_{16}\cdot 0.5C_6H_5Cl$ and $C_{60}\cdot 0.5C_6H_5Cl$ compounds 215 (1993) 137
Kushida, T., see J. Watanabe 213 (1993) 351

Kushida, T., see J.S. Ahn 215 (1993) 336
Kuskov, V.L., see G.G. Lazarev 212 (1993) 319; 215 (1993) 375
Kusumi, T., see K. Yoshikawa 211 (1993) 211
Kuwahara, K., see H. Umemoto 214 (1993) 271
Kwok, A.S., see J.L. Cheung 213 (1993) 309

Laaksonen, L. and J.B. Rosenholm, Molecular dynamics simulations of the water/octanoate interface in the presence of micelles 216 (1993) 429
LaBrake, D. and E. Weitz, H atom mobilities in xenon matrices. Dependence on matrix morphology 211 (1993) 430
Lacks, D.J. and S. Kais, Statistical model for delocalized π bonding in the C_{60} molecule 218 (1994) 229
Lafleur, R.D., see J.M. Parnis 218 (1994) 544
Lagendijk, A., see M.J.P. Brugmans 217 (1994) 117
Lahaye, R.J.W.E., see A.E. Wiskerke 216 (1993) 93
Lahmani, F., A. Douhal, E. Breheret and A. Zehnacker-Rentien, Solvation effects in jet-cooled 7-hydroxyquinoline 220 (1994) 235
Laisaar, A., see A. Freiberg 214 (1993) 10
Laitinen, E., P. Ruuskanen-Järvinen, U. Rempel, V. Helenius and J.E.I. Korppi-Tommola, Rotation correlation time as a measure of microviscosity of excited state isomerization reactions of three cyanine dyes in *n*-alcohol solutions 218 (1994) 73
Lakshminarayana, V., see V. Nagalakshmi 217 (1994) 279
Lamb, L.D., see L. Nemes 218 (1994) 295
Lambert, I.R., see M.D. Wheeler 211 (1993) 381
Lambert, J.M., see P.M. Ajayan 215 (1993) 509
Lami, A., see A. Ferretti 220 (1994) 327
Landman, U., see C. Yannouleas 217 (1994) 175
Landuyt, L., see M.T. Nguyen 212 (1993) 543
Lang, J.M., A.A. Dadali and H.G. Drickamer, Luminescence of the flexible dye molecule julolidinemalononitrile in polymer matrices at pressures above 40 kbar 214 (1993) 310
Langenberg, J.D., see J.C. Pinegar 212 (1993) 458
Langhoff, S.R. and C.W. Bauschlicher Jr., A theoretical study of the electric dipole moment function of SiO 211 (1993) 305
Langhoff, S.R., see C.W. Bauschlicher Jr. 211 (1993) 312; 216 (1993) 341
Langridge-Smith, P.R.R., see A.C. Jones 219 (1994) 174
Lanig, H., M. Hof, T. Stahl and F.W. Schneider, Intramolecular deactivation of substituted quinolinium cations. Time-resolved fluorescence and semi-empirical calculations 220 (1994) 423
Lantz, K.O. and V. Vaida, Direct absorption spectroscopy of the first excited electronic band of jet-cooled H_2S 215 (1993) 329
Lantz, S., see J.V. Gilbert 220 (1994) 19
Lanza, G., see S. Di Bella 214 (1993) 598
Lanzisera, D.V. and J.J. Valentini, Surprising positive correlation between rotational and vibrational excitation in the $H+CDCl_3 \rightarrow HD+CCl_3$ reaction 216 (1993) 122
Lao, K., see H. Guo 218 (1994) 212
Lap, D.V., D. Grebner, S. Rentsch and H. Naarmann, Femtosecond-spectroscopic investigations on bithiophene, terthiophene and tetrathiophene in solution 211 (1993) 135
Lara, F., see G.G. Lazarev 212 (1993) 319
Lardeux-Dedonder, C., see S. Martrenchard-Barra 215 (1993) 291
Larin, A.V., S.V. Poljanskii and D.N. Trubnikov, Assignment of the torsional structure of the 0_0^0 band of the electronic transition $A_{1g} \rightarrow B_{2u}$ in van der Waals clusters of type C_6H_6–X (X=N_2, CO_2, CO) 213 (1993) 619
Larsen, R.G., J. Shore, K. Schmidt-Rohr, L. Emsley, H. Long, A. Pines, M. Janicke and B.F. Chmelka, NMR study of xenon dynamics and energetics in Na–A zeolite 214 (1993) 220
Larsson, J., see P. Erman 215 (1993) 173

Larsson, M., see G. Sundström 218 (1994) 17
Larsson, S., see M. Braga 213 (1993) 217
Last, I., see A. Baram 212 (1993) 649; 215 (1993) 416
Last, I. and T.F. George, Multiple ionization of rare gas clusters. Theoretical treatment 216 (1993) 599
Last, I., see M. Baer 219 (1994) 372
Latajka, Z., see O.N. Ventura 217 (1994) 436
Laubereau, A., see K. Wolfrum 213 (1993) 41
Laubereau, A., see R. Gagel 217 (1994) 228
Lauderdale, W., see R. Pandey 220 (1994) 337
Laukenmann, K., see G.G. Lazarev 215 (1993) 375
Laukien, F.H., see D.G. Cory 212 (1993) 487
Laurent, T., see S. Koppe 214 (1993) 546
Lavrich, D.J., see M.A. Buntine 216 (1993) 471
Law, M.M. and J.L. Duncan, Second-order perturbation theory corrections to effective Fermi resonance coupling constants 212 (1993) 172
Lawley, K.P., see M.C.R. Cockett 214 (1993) 27
Lawley, K.P., see M.S.N. Al-Kahali 220 (1994) 225
Lawrance, W.D., see R.A.J. Borg 218 (1994) 320
Lazarev, G.G., V.L. Kuskov, F. Lara, F. García, A. Rieker and P. Tordo, The role of dopant geometry in the photoinduced formation of radical pairs in crystals of 2,6-di-tert-butyl-4-methylphenol and 2,6-di-tert-butylphenol 212 (1993) 319
Lazarev, G.G., V.L. Kuskov, K. Laukenmann and A. Angerhofer, Spin dynamics of neutral radical pairs in single crystals of di-tert-butyl-pyrocatechol doped with tetrakis(*t*-butyl)-phenoxazin 215 (1993) 375
Lazzeretti, P., M. Malagoli and R. Zanasi, Computational approach to molecular magnetic properties by continuous transformation of the origin of the current density 220 (1994) 299
Leach, C.A., see A. Carrington 212 (1993) 473
Leach, D.H., see J.L. Cheung 213 (1993) 309
Leahy, D.J., D.R. Cyr, D.L. Osborn and D.M. Neumark, Observation of the correlated O $^3P_{j1}$, $^3P_{j2}$ state distribution from the predissociation of O_2 B $^3\Sigma_u^-$ 216 (1993) 503
Lebeault-Dorget, M.A., see R.F. Barrow 214 (1993) 293
Lebedev, Ya.S., see D.S. Tipikin 215 (1993) 199
Lebedev, Ya.S., see S.D. Chemerisov 218 (1994) 353
Leclercq, J.-M., see L. Koubi 217 (1994) 544
Lederer, T., see D. Arvanitis 211 (1993) 53
Lee, C., see C. Sosa 211 (1993) 265
Lee, C.H., see B. Kraabel 213 (1993) 389
Lee, K., J.S. Goo and J.K. Ku, Radiative lifetimes and intramultiplet mixing rate constants for Ga(4d) atoms in Ar 216 (1993) 483
Lee, M.-T., see K. Wang 219 (1994) 397
Lee, S., see K.S. Kim 216 (1993) 309
Lee, S.J., see J. Kim 219 (1994) 243
Lee, T.J., see R. Kobayashi 211 (1993) 94
Lee, T.J., A coupled-cluster study of HNO_2 and FNO_2 216 (1993) 194
Lee, T.J., see R.J. Rico 218 (1994) 139
Lee, T.J., see M. Head-Gordon 219 (1994) 21
Lee, Y.R., C.L. Chiu and S.M. Lin, Photodissociation of S_2Cl_2 at 308 nm by translational spectroscopy 216 (1993) 209

Lee, Y.T., see D.W. Boo 211 (1993) 358
Leegwater, J.A. and S. Mukamel, Four-wave mixing signatures of exciton Bose condensation 217 (1994) 456
Legay, F. and N. Legay-Sommaire, NO diffusion and dimer formation in a nitrogen matrix studied by FTIR spectroscopy 211 (1993) 516
Legay, F., see N. Legay-Sommaire 217 (1994) 97
Legay-Sommaire, N., see F. Legay 211 (1993) 516
Legay-Sommaire, N. and F. Legay, Photochemical formation of CH_3HgH in $Hg/CH_4/Ar$ matrices studied by FTIR spectroscopy 217 (1994) 97
Legon, A.C. and J.C. Thorn, Equilibrium nuclear quadrupole coupling constants from the rotational spectrum of BrCl: a source of the electric quadrupole moment ratios $Q(^{79}Br)/Q(^{81}Br)$ and $Q(^{35}Cl)/Q(^{37}Cl)$ 215 (1993) 554
Leininger, T., J.-F. Riehl, G.-H. Jeung and M. Pélissier, Reply to Comment on "Comparison of the widely used HF pseudo-potentials: MH^+ (M=Fe, Ru, Os)" 220 (1994) 345
Lelj, F., see G. Ricciardi 215 (1993) 541
Lemaire, J., see S. Jullien 212 (1993) 340
Lemoine, P., K. Cazzini, I.T. McGovern, W.J. Blau, P. Bätz, C. Ziegler and W. Göpel, X-ray photoelectron spectroscopy of KrF laser-irradiated polycarbonate films 220 (1994) 177
Lenderink, E., K. Duppen and D.A. Wiersma, Femtochemistry of the iodine–arene charge-transfer complex 211 (1993) 503
Lenderink, E. and D.A. Wiersma, Photodissociation dynamics of dimethylnitrosamine studied by resonance Raman spectroscopy 218 (1994) 586
Leone, S.R., see S.D. Price 214 (1993) 553
Lequan, M., R.M. Lequan, K.C. Ching, M. Barzoukas, A. Fort, G. Bravic, D. Chasseau, Y. Barrans and M. Huché, Quadratic non-linear optical properties of N-(4-nitrostilbenyl) (S) prolinol 213 (1993) 71
Lequan, R.M., see M. Lequan 213 (1993) 71
Lermé, J., see M. Pellarin 217 (1994) 349
Lesyng, B., see P. Bala 219 (1994) 259
Letokhov, V.S., see I.V. Bezel 218 (1994) 475
Leung, K.T., see J.F. Ying 212 (1993) 289
Levanon, H., see A. Berman 211 (1993) 549
Levine, R.D., see M. Ben-Nun 214 (1993) 175; 220 (1994) 291
Levine, R.D., see K.L. Bintz 215 (1993) 455
Levine, Y.K., see D.A. van der Sijs 216 (1993) 559
Lewis, T.A., see L.D. Hulett Jr. 216 (1993) 236
Leyte, J.C., see T.W.N. Bieze 216 (1993) 56
Li, B., N.C. Bartelt and E.D. Williams, The contact angles of trapped steps 217 (1994) 595
Li, F., see L. Xu 212 (1993) 265
Li, F.-E, see R.-J. Li 220 (1994) 281
Li, H., see Q. Zhu 212 (1993) 403
Li, H.-W., see T.-C. Chang 213 (1993) 564
Li, J., see P. Pyykkö 218 (1994) 133
Li, M., see J.P. Culver 214 (1993) 431
Li, Q. and L. Luo, The kinetic theory of thermal hysteresis of a macromolecule solution 216 (1993) 453
Li, Q.-S., see A.-C. Tang 212 (1993) 391
Li, R.-J., K.-L. Han, F.-E Li, R.-C. Lu, G.-Z. He and N.-Q. Lou, Rotational alignment of product molecules from the reactions $Sr+CH_3Br$, C_2H_5Br, n-C_3H_7Br, i-C_3H_7Br by means of PLIF 220 (1994) 281

Li, S., see Y. Chen 211 (1993) 449
Li, S., see R.J. Van Zee 217 (1994) 381
Li, W.-K., see N.L. Ma 213 (1993) 189, 250
Li, Y., M. Honigmann, G. Hirsch and R.J. Buenker, Theoretical study of line broadening in the $(3s\sigma)\ ^3\Pi_g$ vibrational levels of the O_2 molecule employing a diabatic CI representation 212 (1993) 185
Li, Z., see J.S. Francisco 214 (1993) 77, 591
Li, Z., A. Borrmann and C.C. Martens, Wavelet analysis of condensed phase molecular dynamics 214 (1993) 362
Li, Z., see R. Zadoyan 218 (1994) 504
Li, Z., see R. Liu 219 (1994) 143
Liao, C.-L., see Z.-X. Ma 213 (1993) 250
Liao, D.-W. and K. Balasubramanian, Germanium monochloride (GeCl). Spectroscopic constants and potential energy curves 213 (1993) 174
Lichanot, A. and M. Rerat, Elastic properties in BeO. An ab initio Hartree–Fock calculation 211 (1993) 249
Liddell, M.J., see P. Schwerdtfeger 218 (1994) 362
Liebermann, H.-P., I. Boustani, S.N. Rai, A.B. Alekseyev, G. Hirsch and R.J. Buenker, Use of relativistic core potentials to compute potential curves and lifetimes of low-lying states of arsenic fluoride 214 (1993) 381
Lienau, Ch., J.C. Williamson and A.H. Zewail, Femtochemistry at high pressures. The dynamics of an elementary reaction in the gas–liquid transition region 213 (1993) 289
Light, J.C., see D.E. Manolopoulos 216 (1993) 18
Lim, E.C., see H. Saigusa 211 (1993) 410
Lim, S.K., M.E. Burba and A.C. Albrecht, The Stokes law radius of the C_{60} radical anion in *n*-hexane by time-of-flight mobility measurements 216 (1993) 405
Lin, S.H., see M. Hayashi 213 (1993) 465
Lin, S.H., see B. Fain 216 (1993) 551
Lin, S.M., see Y.R. Lee 216 (1993) 209
Lin, Z., K. Boraas and J.P. Reilly, The vibrational overtone spectrum of fluoroform in the $\Delta v = 4$ C–H stretching region 217 (1994) 239
Linnartz, H., see G. Hilpert 219 (1994) 384
Liou, H.T., see B. Fain 216 (1993) 551
Liu, A., see D.A. Dolson 212 (1993) 118
Liu, F., S.H. Garofalini , R.D. King-Smith and D. Vanderbilt, Structural and electronic properties of sodium metasilicate 215 (1993) 401
Liu, K., see Z. Ma 213 (1993) 269
Liu, L., see H. Guo 218 (1994) 212
Liu, R. and X. Zhou, Comment on "Cyclopentadienylideneketene: theoretical confirmation of a key infrared band" 212 (1993) 702
Liu, R., S. Ma and Z. Li, Theoretical study on the dynamic properties and state-selected rate constants of the reaction $CH(^4\Sigma^-) + H_2 \rightarrow CH_2(^3B_1) + H$ 219 (1994) 143
Liu, X.-Y., P. Bennema, L.A. Meijer and M.S. Couto, Ordering of paraffin-like molecules at the solid–fluid interface 220 (1994) 53
Liu, Y., see P.B. Davies 214 (1993) 305
Liu, Z., see P.B. Davies 214 (1993) 305
Liyanage, R., P.T.A. Reilly, Y. Yang, R.J. Gordon and R.W. Field, Evidence of the indirect predissociation of the $F\ ^1\Delta$ state of HCl 216 (1993) 544

Locht, R., see J. Momigny 211 (1993) 161
Loesch, H.-J., see M. Baer 219 (1994) 372
Lögdlund, M., see M. Fahlman 214 (1993) 327
Long, H., see R.G. Larsen 214 (1993) 220
Longo, R., A. Diz, E. Deumens and Y. Öhrn, Influence of electronic–nuclear coupling on dynamics 220 (1994) 305
Loo, B.H., Enhanced Raman scattering from hexacyanoferrate (II) and (III) ions adsorbed on silver electrode surfaces 213 (1993) 479
Loos, M., see J.G. Ángyán 219 (1994) 267
Lossing, F.P., see J.L. Holmes 212 (1993) 134
Lou, L., see J.A. Mares 217 (1994) 105
Lou, N., see Z. Song 217 (1994) 142
Lou, N., see G. Ding 220 (1994) 1
Lou, N.-Q., see R.-J. Li 220 (1994) 281
Loutellier, A., see S. Coussan 217 (1994) 123
Lu, R., see Z. Song 217 (1994) 142
Lu, R.-C., see R.-J. Li 220 (1994) 281
Lubitz, W., see A. Van der Est 212 (1993) 561
Lucas, J.M., see A. Aguilar 220 (1994) 267
Lüchow, A., R. Barrois and H. Kleindienst, Accurate nonrelativistic energies for the lowest ^4S states of Li 216 (1993) 359
Lüchow, A., see H. Kleindienst 218 (1994) 441
Luckhaus, D., M. Quack and J. Stohner, Femtosecond quantum structure, equilibration and time reversal for the CH-chromophore dynamics in CHD_2F 212 (1993) 434
Luckhurst, G.R., see A. Ferrarini 214 (1993) 409
Lugez, C., see L. Schriver-Mazzuoli 214 (1993) 519
Lund, A., see N.P. Benetis 218 (1994) 551
Lundqvist, B.I., see C. Engdahl 215 (1993) 103
Luo, L., see Q. Li 216 (1993) 453
Luo, Y., H. Ågren, S. Knuts and P. Jørgensen, The two-photon spectrum of pyrimidine. Role of vibronic coupling 213 (1993) 356
Lynch, G.C., see S.L. Mielke 213 (1993) 10; 216 (1993) 441; 217 (1994) 173
Lynden-Bell, R.M., see L.D. Gelb 211 (1993) 328

Ma, N.L., S.S. Wong, M.N. Paddon-Row and W.-K. Li, Is HPC a minimum on the HCP potential surface? A failure of the Møller–Plesset perturbation theory 213 (1993) 189
Ma, N.L., see Z.-X. Ma 213 (1993) 250
Ma, S., see R. Liu 219 (1994) 143
Ma, X., see Y. Chen 211 (1993) 449
Ma, Y., see M. Neeb 212 (1993) 205
Ma, Z. and K. Liu, Collision-induced fine-structure transition of $O(^3P_2) \rightarrow O(^3P_{1,0})$ by He and H_2: excitation function and branching ratio 213 (1993) 269
Ma, Z.-X., C.-L. Liao, H.-M. Yin, C.Y. Ng, S.-W. Chiu, N.L. Ma and W.-K. Li, Experimental and theoretical studies of isomeric C_2H_5S and $C_2H_5S^+$ 213 (1993) 250
Maas, W.E., see D.G. Cory 212 (1993) 487
Mac, M. and J. Wirz, Deriving intrinsic electron-transfer rates from nonlinear Stern–Volmer dependencies for fluorescence quenching of aromatic molecules by inorganic anions in acetonitrile 211 (1993) 20
MacPhail, R.A., see X. Pan 212 (1993) 64
Mäder, H., see H. Harder 214 (1993) 265
Maeda, M., see K. Sakoda 217 (1994) 152
Maekawa, K., see Y. Kohno 214 (1993) 603
Mafuné, F., J. Kohno, T. Nagata and T. Kondow, Mechanism of ion ejection from a liquid beam following laser photoionization 218 (1994) 7
Mafuné, F., Y. Takeda, T. Nagata and T. Kondow, Inhomogeneous solvation in an aniline–ethanol solution studied by laser photoionization of a liquid beam 218 (1994) 234
Magnasco, V., A. Siciliano and G. Figari, Variationally improving the Inui wavefunction for H_2 213 (1993) 17
Magnera, T.F., D.M. Sammond and J. Michl, Ground-state rotational constants of Ar_3^+ by rotational depletion coherence spectroscopy 211 (1993) 378
Magni, V., see M. Nisoli 220 (1994) 64
Mahajan, A., see L.A. Keeling 217 (1994) 136
Mahgoub, A.S., see N.P. Benetis 218 (1994) 551
Mahi, L., J.C. Duplan and B. Fenet, Suppression of *J*-modulation effects for resonance editing by NMR spin-echo experiments 211 (1993) 27
Mai, J., A. Casties and W. von Niessen, A Monte Carlo simulation for the catalytic oxidation of CO on DLA clusters 211 (1993) 197
Maier, J.P., see M. Fehér 211 (1993) 171
Maier, J.P., see J. Fulara 211 (1993) 227
Maiti, A., see C.J. Brabec 219 (1994) 473
Maity, D.K., see H. Mohan 220 (1994) 455
Majchrzak, I., see N.D. Kushch 215 (1993) 137
Makarov, V.I., see S.A. Nizkorodov 215 (1993) 662
Malagoli, M., see P. Lazzeretti 220 (1994) 299
Malicet, J., see J. Brion 213 (1993) 610
Malrieu, J.P., see J. Meller 218 (1994) 276
Malrieu, J.P., see À. Povill 218 (1994) 283
Maltsev, V.A., O.A. Nerushev, S.A. Novopashin and B.A. Selivanov, Anomalous polarizability of fullerene 212 (1993) 480
Maluendes, S.A., A.D. McLean and E. Herbst, New calculations on the ion–molecule processes $C_2H_2^+ + H_2 \rightarrow C_2H_3^+ + H$ and $C_2H_2^+ + H_2 \rightarrow C_2H_4^+$ 217 (1994) 571

Mandel, T., see G. Remmers 214 (1993) 241
Mank, A., D. Rodgers and J.W. Hepburn, Threshold photoelectron spectroscopy of HF 219 (1994) 169
Manning, M., see S.D. Price 214 (1993) 553
Manolopoulos, D.E. and J.C. Light, A log derivative formulation of reaction rate theory 216 (1993) 18
Mansfeld, M. and W.S. Veeman, The use of ^{129}Xe NMR exchange spectroscopy for probing the microstructure of porous materials 213 (1993) 153
Manthe, U. and A.D. Hammerich, Wavepacket dynamics in five dimensions. Photodissociation of methyl iodide 211 (1993) 7
Mao, X., J. Guo and C. Ye, Competition between radiation damping and transverse relaxation effects on NMR signal intensities 218 (1994) 249
Marco, P.D., see G. Giro 211 (1993) 580
Marconi, G., see G. Giro 211 (1993) 580
Marecek, J., see Q. Ying 219 (1994) 214
Mares, J.A., G. Boulon, A. Brenier, L. Lou and S.R. Rotman, Spectroscopy of multisites Cr^{3+} and Nd^{3+} in yttrium aluminum perovskite 217 (1994) 105
Maresch, G.G., see M. Hubrich 218 (1994) 81
Marian, C.M., Stability and the CO stretching vibrational frequency of molecular AgCO 215 (1993) 582
Maricq, M.M. and J.J. Szente, Upper limits for the rate constants of the reactions $CF_3O+O_3 \rightarrow CF_3O_2+O_2$ and $CF_3O_2+O_3 \rightarrow CF_3O+2O_2$ 213 (1993) 449
Maricq, M.M. and J.J. Szente, One- and two-photon dissociation of acetyl chloride at 193 nm 220 (1994) 243
Märk, T.D., see D. Smith 213 (1993) 202
Märk, T.D., see M. Kolibiar 219 (1994) 252
Märk, T.D., see P. Scheier 220 (1994) 141
Marks, A.J., see B.R. Eggen 219 (1994) 247
Marr, A.J., see A. Carrington 212 (1993) 473
Martens, C.C., see L.M. Finney 214 (1993) 159
Martens, C.C., see Z. Li 214 (1993) 362
Martens, C.C., see R. Zadoyan 218 (1994) 504
Mårtensson, N., see P.A. Brühwiler 214 (1993) 45
Martin, P.A., see M. Fehér 215 (1993) 565
Martinez, M.L., see P.-T. Chou 220 (1994) 229
Martinho, J.M.G., see A.T. Reis e Sousa 213 (1993) 333
Martrenchard-Barra, S., C. Jouvet, C. Lardeux-Dedonder and D. Solgadi, Molecular dynamics simulations of the formation process of very small doubly charged para-difluorobenzene clusters produced in a supersonic expansion 215 (1993) 291
Maruyama, K., see A. Osuka 215 (1993) 179
Maruyama, Y., see E. Frankevich 214 (1993) 39
Maruyama, Y., see M. Ishikawa 219 (1994) 416
Marx, R., see S. Jullien 212 (1993) 340
Masaki, A., S. Tsunashima and N. Washida, Rate constant for the reaction of CH_3O_2 with NO 218 (1994) 523
Masaki, N.M., see Y. Fujitani 214 (1993) 301
Mason, J., see P.J. Barrie 219 (1994) 491
Mastenbroek, J.W.G., see C.A. Taatjes 216 (1993) 100
Mastromarino, J., see U.K.A. Klein 217 (1994) 80, 86
Masuhara, H., see N. Tamai 211 (1993) 364

Masuhara, H., see S. Hamai 213 (1993) 407
Masuhara, H., see S. Yamamoto 215 (1993) 323
Masuhara, H., see S. Hashimoto 219 (1994) 445
Masuhara, H., see N. Fukazawa 220 (1994) 461
Mataga, N., see A. Osuka 215 (1993) 179
Mathers, C.P., see J.F. Ying 212 (1993) 289
Mathur, D., see M. Krishnamurthy 216 (1993) 203
Mathur, D., see G.R. Kumar 217 (1994) 626
Matsui, T., see J. Ishii 220 (1994) 29
Matsumi, Y., see M. Ohashi 220 (1994) 7
Matsumura, T., see Y. Mori 211 (1993) 421
Matsuo, T., see Y. Miyazaki 213 (1993) 303
Matsuoka, M., see J. Takeda 220 (1994) 443
Matsuoka, O., Reply to Comment on "Segmented contractions of relativistic Gaussian basis sets" 212 (1993) 550
Matsushita, M., A.M. Frens, E.J.J. Groenen, O.G. Poluektov, J. Schmidt, G. Meijer and M.A. Verheijen, Triplet excitations of crystalline C_{60}. An optically detected magnetic-resonance study in zero field 214 (1993) 349
Matsuzaki, S.Y., see S. Murata 219 (1994) 200
Matsuzaki, Y., K. Tanaka and T. Yamabe, Electronic excitations to higher two-photon states of conjugated polymers 211 (1993) 300
Mattar, S.M. and B.J. Doleman, MRSD-CI and LDF studies of the VN X $^3\Delta$ and D $^3\Pi$ states 216 (1993) 369
Matveets, Yu.A., see I.V. Bezel 218 (1994) 475
Matveev, A.A., A.M. Pravilov and A.F. Vilesov, Anomalously large isotope effect in the chemiluminescence from $N(^4S)+O(^3P)$ recombination 217 (1994) 582
Matyushov, D.V. and R. Schmid, Stationary points in the temperature dependence of electron transfer rates 220 (1994) 359
Mauclaire, G., see S. Jullien 212 (1993) 340
Mavridis, A., see A. Papakondylis 216 (1993) 167
May, B.D., see S.F. Cartier 220 (1994) 23
Mayer, E., see G. Fleissner 218 (1994) 93
Mayer, I., see B. Paizs 220 (1994) 97
Mayer, P.M., see J.L. Holmes 212 (1993) 134
Maynau, D. and J.-L. Heully, Second-order perturbation on a SDCI calculation 211 (1993) 625
McBranch, D., see B. Kraabel 213 (1993) 389
McCaffery, A.J., see C.M. Quintella 214 (1993) 563
McCammon, J.A., see P. Bala 219 (1994) 259
McClean, R.E. and L. Pasternack, Kinetics of the reactions $VO(X\ ^4\Sigma^-)+O_2$, NO, and CO_2 215 (1993) 209
McCormack, E.F., S.T. Pratt, P.M. Dehmer and J.L. Dehmer, Double-resonance laser-induced grating spectroscopy of nitric oxide 211 (1993) 147
McDonald, I.R., see K.D. Hammonds 213 (1993) 27
McDonald, I.R., see M. Ferrario 213 (1993) 537
McDowell, A.F., see S. Miyajima 212 (1993) 277
McDowell, C.A., see T. Nakai 217 (1994) 234
McFeaters, J.S., see P. Schwerdtfeger 218 (1994) 362
McGibbon, G.A., P.C. Burgers and J.K. Terlouw, O-protonated sulfine CH_2=S=OH^+. Its generation from ionized dimethylsulfoxide by delayed dissociation 218 (1994) 499

McGlynn, S.P., see U. Asaf 212 (1993) 326
McGovern, I.T., see P. Lemoine 220 (1994) 177
McGowen, J.L., see J.Z. Zhang 218 (1994) 479
McKee, M.L., Theoretical study of the CH_3SOO radical 211 (1993) 643
McKoy, V., see J.F. Ying 212 (1993) 289
McKoy, V., see K. Wang 217 (1994) 490; 219 (1994) 397
McLauchlan, K.A., see S.N. Batchelor 214 (1993) 507
McLauchlan, K.A., I.A. Shkrob and M.T. Yeung, Room-temperature observations of spin-polarized triplet anthracene 217 (1994) 157
McLean, A.D., see S.A. Maluendes 217 (1994) 571
McLuckey, S.A., see L.D. Hulett Jr. 216 (1993) 236
McMullen, T., see M. Rabinowitz 218 (1994) 437
Mebel, A.M., D.G. Musaev and K. Morokuma, Ab initio molecular orbital study of structure and NMR ^{11}B chemical shifts of Lewis base adducts of CO, NH_3, PF_3, and PH_3 with small nido-boranes, B_3H_7 and B_4H_8 214 (1993) 69
Mebel, A.M., D.G. Musaev and K. Morokuma, An alternative mechanism of BH_2SH formation in the reaction of B_2H_6 with SH_2: concerted elimination of BH_3 and H_2 from $H_2S{\cdot}B_2H_6$. Ab initio MO study 216 (1993) 313
Medikeri, M.N. and M.K. Mishra, Quasiparticle approximation to the dilated electron propagator with application to ^2P shape resonances in e–Be and e–Ca scattering 211 (1993) 607
Medina, A., see J.M.M. Roco 216 (1993) 593
Meerts, W.L., see G. Hilpert 219 (1994) 384
Meier, B.H., see S. Hediger 213 (1993) 627
Meier, B.H., see M. Tomaselli 214 (1993) 1
Meier, Ch. and V. Engel, Electron kinetic energy distributions from multiphoton ionization of Na_2 with femtosecond laser pulses 212 (1993) 691
Meijer, G., see M. Matsushita 214 (1993) 349
Meijer, G., see M.A. Verheijen 216 (1993) 72
Meijer, G., M.G.H. Boogaarts, R.T. Jongma, D.H. Parker and A.M. Wodtke, Coherent cavity ring down spectroscopy 217 (1994) 112
Meijer, G., see J.L. de Boer 219 (1994) 469
Meijer, L.A., see X.-Y. Liu 220 (1994) 53
Meissner, L., A. Balková and R.J. Bartlett, Multiple solutions of the single-reference coupled-cluster method 212 (1993) 177
Meller, J., J.L. Heully and J.P. Malrieu, Size-consistent self-consistent combination of selected CI and perturbation theory 218 (1994) 276
Melroy, O.R., see W. Schmickler 216 (1993) 424
Menon, M. and K.R. Subbaswamy, Structure of Si_{60}. Cage versus network structures 219 (1994) 219
Menon, S.V.G., see P.S. Goyal 211 (1993) 559
Menzel, H., see Z. Sekkat 220 (1994) 497
Merchán, M., see L. Serrano-Andrés 211 (1993) 125
Merckens, H.-P., see H. Kleindienst 218 (1994) 441
Mercouris, T., see C.A. Nicolaides 212 (1993) 685
Mesbah, S., see Z.D. Popovic 215 (1993) 636
Meskers, S.C.J., J.P. Riehl and H.P.J.M. Dekkers, Linearly polarized luminescence spectra of Eu(2,6-pyridine-dicarboxylate)$_3^{3-}$ in hydroxylic solution 216 (1993) 241
Messaddeq, Y., see S.J.L. Ribeiro 220 (1994) 214

Mestechkin, M.M. and G.E. Whyman, Time-dependent Hartree–Fock theory: finite-field technique for calculation of the Pockels and Kerr effects and generation of harmonics 214 (1993) 144
Metcalf, D.H., see J.P. Bolender 213 (1993) 131
Meyer, E., see J.K. Gimzewski 217 (1994) 589
Mharzi, B., see R. Azria 220 (1994) 417
Mhin, B.J., J. Kim and K.S. Kim, Entropy-driven structures of the hexaaqua-sodium(I) 216 (1993) 305
Mhin, B.J., see K.S. Kim 216 (1993) 309; 219 (1994) 243
Mialocq, J.-C., see P. Hébert 213 (1993) 345
Michael Hollas, J., see R.D. Gordon 211 (1993) 392
Michels, H.H., see J.A. Montgomery Jr. 220 (1994) 391
Michl, J., see T.F. Magnera 211 (1993) 378
Michl, J., see H.S. Plitt 213 (1993) 158
Mielke, S.L., G.C. Lynch, D.G. Truhlar and D.W. Schwenke, A more accurate potential energy surface and quantum mechanical cross section calculations for the $F+H_2$ reaction 213 (1993) 10
Mielke, S.L., G.C. Lynch, D.G. Truhlar and D.W. Schwenke, A separable rotation approximation for the calculation of chemical reaction rates 216 (1993) 441
Mielke, S.L., G.C. Lynch, D.G. Truhlar and D.W. Schwenke, A more accurate potential energy surface and quantum mechanical cross section calculations for the $F+H_2$ reaction (Chem. Phys. Letters 213 (1993) 10). Erratum 217 (1994) 173
Miguel, B., see J.M. García de la Vega 212 (1993) 420
Mihokova, E., see M. Nikl 220 (1994) 14
Mikami, N., see S. Tanabe 215 (1993) 347
Mikhaylova, V.A., see A.I. Ivanov 212 (1993) 697
Miki, H., S. Kimachi, R. Satomi, T. Azumi and M. Onishi, Zero-field splittings of the ligand localized $^3\pi\pi^*$ phosphorescence of the Ru(II) complex with the π-conjugated ligand 218 (1994) 563
Miki, S., see T. Nakayama 213 (1993) 581; 220 (1994) 219
Miklós, A., see M. Fehér 211 (1993) 171
Mikušík, P. and Š. Pick, Tight-binding study of the electronic structure of Pd and Pt epitaxial overlayers on hcp transition metal surfaces 215 (1993) 319
Miller, J., see M. Pellarin 217 (1994) 349
Miller, R.J.D., see S. Astilean 219 (1994) 95
Miller, W.H., see R. Hernandez 214 (1993) 129
Miller, W.H., see S. Keshavamurthy 218 (1994) 189
Mimuro, M., Y. Nishimura, S. Takaichi, Y. Yamano, M. Ito, S. Nagaoka, I. Yamazaki, T. Katoh and U. Nagashima, The effect of molecular structure on the relaxation processes of carotenoids containing a carbonyl group 213 (1993) 576
Minaev, B. and H. Ågren, The interpretation of the Wulf absorption band of ozone 217 (1994) 531
Ming, L., S. Nordholm, G. Nyman and J. Davidsson, Monte Carlo simulation study of statistical limits for energy transfer in binary molecular collisions 211 (1993) 189
Minke, M.A., see S. Seraphin 217 (1994) 191
Minoshima, K., M. Taiji, K. Misawa and T. Kobayashi, Femtosecond nonlinear optical dynamics of excitons in J-aggregates 218 (1994) 67
Minoshima, K., see K. Misawa 220 (1994) 251
Minyaev, R.M. and D.J. Wales, Gradient line reaction path of HF addition to ethylene 218 (1994) 413
Misaizu, F., see H. Umemoto 214 (1993) 271
Misawa, K., see K. Minoshima 218 (1994) 67
Misawa, K., K. Minoshima, H. Ono and T. Kobayashi, Giant static dipole moment change on electronic excitation in highly oriented J-aggregates 220 (1994) 251

Mishra, M.K., see M.N. Medikeri 211 (1993) 607
Misra, T.N., see A.K. Dutta 212 (1993) 637
Mitrushenkov, A.O., Passing the several billions limit in FCI calculations on a mini-computer 217 (1994) 559
Mittal, J.P., see Awadhesh Kumar 212 (1993) 103
Mittal, J.P., see P.K. Chowdhury 218 (1994) 60
Mittal, J.P., see H. Mohan 220 (1994) 455
Mittelbach, A., see L. Akselrod 212 (1993) 384
Mittelbach, A., see K. Kamarás 214 (1993) 338
Miyajima, S., A.F. McDowell and R.M. Cotts, Pulsed-field-gradient stimulated-spin-echo NMR study of anisotropic self-diffusion in smectic Ad liquid crystal CBOOA 212 (1993) 277
Miyatake, Y., see H. Hase 215 (1993) 141
Miyazaki, T., see Y. Fujitani 214 (1993) 301
Miyazaki, T., K. Yamamoto and J. Arai, Effect of rotational quantum states ($J=0, 1$) of matrix H_2 molecules on ESR spectra of radicals at 4.2 K 219 (1994) 405
Miyazaki, Y., T. Matsuo and H. Suga, Glass transition of myoglobin crystal 213 (1993) 303
Mizuki, J., see K. Tanigaki 213 (1993) 395
Mizuma, H., see S. Yamamoto 215 (1993) 323
Mó, O., M. Yáñez, I. Rozas and J. Elguero, Structure, vibrational frequencies and thermodynamic properties of hydrogen peroxide–water dimers. An ab initio molecular orbital study 219 (1994) 45
Möbius, K., see S.D. Chemerisov 218 (1994) 353
Modesti, S., see J.K. Gimzewski 213 (1993) 401
Moerner, W.E., see P. Tchénio 213 (1993) 325
Mohammad, F., see V.R. Morris 220 (1994) 448
Mohan, H., D.K. Maity and J.P. Mittal, Effect of fluorine substitution on the $^{\cdot}OH$-radical-induced electron-transfer reaction in aqueous solutions of fluorinated alkyl iodides 220 (1994) 455
Moine, B., see C. Pédrini 220 (1994) 433
Molin, Yu.N. and K.M. Salikhov, Spin exchange interaction as a possible source of oscillations in recombination of spin-correlated radical pairs 211 (1993) 484
Møller, S.P., see L.H. Andersen 217 (1994) 204
Momicchioli, F., see M. Caselli 216 (1993) 41
Momigny, J. and R. Locht, The appearance of $C_2H_3^+$ ions from C_2H_3F by non-resonant photoionization. A translational energy surprisal analysis 211 (1993) 161
Monks, P.S., L.J. Stief, M. Krauss, S.C. Kuo and R.B. Klemm, A discharge-flow photoionization mass-spectrometric study of the $BrO(X\ ^2\Pi)$ radical. Photoionization spectrum and ionization energy 211 (1993) 416
Montgomery Jr., J.A., H.H. Michels and J.S. Francisco, Ab initio calculation of the heats of formation of CF_3OH and CF_2O 220 (1994) 391
Moore, E.A., see P.J. Barrie 219 (1994) 491
Moore, J.H., see D.C. Winkler 219 (1994) 57
Mori, A., see H. Sekiya 215 (1993) 641
Mori, W., see M. Okumura 219 (1994) 36
Mori, Y., Y. Nakamichi, T. Sekiguchi, N. Okazaki, T. Matsumura and I. Hanazaki, Photoinduction of chemical oscillation in the Belousov–Zhabotinsky reaction under the flow condition 211 (1993) 421
Mori, Y., see T. Sekiguchi 219 (1994) 81
Morikawa, E., see M. Chergui 216 (1993) 34

Morikawa, T., see A. Ito 211 (1993) 333
Morley, G.P., P. Felder and J.R. Huber, Photodissociation of dichlorocarbene CCl_2 at 248 nm in a cold beam 219 (1994) 195
Morokuma, K., see A.M. Mebel 214 (1993) 69; 216 (1993) 313
Morozov, A.K., see M.M. Triebel 214 (1993) 321
Morris, R.C., see R.C. Haddon 218 (1994) 100
Morris, V.R., F. Mohammad, L. Valdry and W.M. Jackson, Steric effects on nascent vibrational distributions of the HCN product produced in CN radical reactions with ethane, propane and chloroform 220 (1994) 448
Morse, M.D., see J.C. Pinegar 212 (1993) 458
Morton, J.R., F. Negri and K.F. Preston, The EPR spectra of hydrides of C_{70}. An experimental and theoretical investigation 218 (1994) 467
Moses, D., see C. Halvorson 212 (1993) 85
Moses, D., see B. Kraabel 213 (1993) 389
Mostafavi, M., see S. Remita 218 (1994) 115
Motyakin, M.V. and N.G. Spitchina, ESR study of the fullerene C_{60} under axial and shear deformation 216 (1993) 63
Mudjijono, see R.A.J. Borg 218 (1994) 320
Mujica, V., see J.L. Paz 217 (1994) 333
Mukai, K., K. Nedachi, J.B. Jamali and N. Achiwa, Magnetic properties of 1,5-dimethylverdazyl radicals. I. Evidence for the ferromagnetic exchange interaction in 3-(4-chlorophenyl)-1,5-dimethyl-6-thioxoverdazyl radical solid 214 (1993) 559
Mukai, M., see Y. Fujiwara 213 (1993) 89
Mukaihata, H., T. Ohkubo, Y. Fujiwara and M. Itoh, Picosecond time-resolved fluorescence of the intramolecular excited-state proton transfer in 2-naphthyl-3-hydroxychromones. Torsional relaxation in the excited states 211 (1993) 140
Mukamel, S., see A. Takahashi 216 (1993) 394
Mukamel, S., see J.A. Leegwater 217 (1994) 456
Mukherjee, P.K., see T.K. Ghosh 218 (1994) 433
Mukoyama, T. and H. Adachi, Electronic structures of d^0 complexes by the DV-Xα method 215 (1993) 93
Mukoyama, T., see J. Onoe 217 (1994) 61
Müller, G., see J. Hohmann 217 (1994) 577
Müller, H., see M. Schmitt 218 (1994) 246
Müller, S.C., see B. Neumann 211 (1993) 36
Müller, W.H., see A. Angerhofer 217 (1994) 403
Mundschau, M., see B. Rausenberger 215 (1993) 109
Muñoz, L.A., see X. Gu 211 (1993) 65
Murad, E., see R.A. Dressler 215 (1993) 656
Murata, K., see N. Hatta 217 (1994) 398
Murata, S., M. Nishimura, S.Y. Matsuzaki and M. Tachiya, Transient effect in fluorescence quenching induced by electron transfer. I. Analysis by the Collins–Kimball model of diffusion-controlled reactions 219 (1994) 200
Murrell, J.N., see B.R. Eggen 219 (1994) 247
Murry, R.L., see D.L. Strout 214 (1993) 576
Musaev, D.G., see A.M. Mebel 214 (1993) 69; 216 (1993) 313
Müschenborn, H.-J., see M. Croci 212 (1993) 71
Muthu, D.V.S., M.N. Shashikala, A.K. Sood, R. Seshadri and C.N.R. Rao, Raman study of the doped fullerene C_{60}·TDAE 217 (1994) 146

Myers, A.B., see R. Zhang 211 (1993) 541
Myers, A.B., see P. Tchénio 213 (1993) 325
Mys, G., see A. Ceulemans 219 (1994) 274

Naaman, R., see Y. Hurwitz 215 (1993) 674
Naarmann, H., see D.V. Lap 211 (1993) 135
Nabedryk, E., see J. Breton 213 (1993) 571
Nadjo, L., see B. Keita 215 (1993) 125
Nagalakshmi, V., V. Lakshminarayana, G. Sumithra and M. Durga Prasad, Coupled cluster description of anharmonic molecular vibrations. Application to O_3 and SO_2 217 (1994) 279
Nagaminé, M., see T. Tsukuda 218 (1994) 1
Nagano, Y., T. Kiyobayashi and T. Nitta, CO_2 absorption in C_{60} solid 217 (1994) 186
Naganuma, T., see K. Hoshino 211 (1993) 571
Naganuma, T., see A. Nakajima 214 (1993) 22
Nagao, H., K. Nishikawa and S. Aono, The Hückel model by means of the path integral method. II. Application to the square lattice system 215 (1993) 5
Nagaoka, S., see M. Mimuro 213 (1993) 576
Nagase, S. and K. Kobayashi, Metallofullerenes MC_{82} (M=Sc, Y, and La). A theoretical study of the electronic and structural aspects 214 (1993) 57
Nagashima, U., see M. Mimuro 213 (1993) 576
Nagata, T., see T. Tsukuda 218 (1994) 1
Nagata, T., see F. Mafuné 218 (1994) 7, 234
Nagayama, K., see T. Fujiwara 212 (1993) 81
Nagy, G. and D. Roy, Surface charge dependence of second harmonic generation from a Ni electrode 214 (1993) 197
Nagy-Ungvarai, Zs., see B. Neumann 211 (1993) 36
Naik, P.D., see S. Koppe 214 (1993) 546
Nair, K.P.R., see J. Hoeft 215 (1993) 371
Nair, P.G., see K.B. Ghose 211 (1993) 15
Nakabayashi, S. and K. Uosaki, Synchronization of electrochemical oscillations with external perturbations 217 (1994) 163
Nakahara, J., see J. Watanabe 213 (1993) 351
Nakahara, N., see K. Kikuchi 216 (1993) 67
Nakai, T. and C.A. McDowell, Residual chemical-shift effects in spin-echo NMR powder patterns of homonuclear dipolar-coupled spins 217 (1994) 234
Nakajima, A., see K. Hoshino 211 (1993) 571
Nakajima, A., T. Taguwa, K. Hoshino, T. Sugioka, T. Naganuma, F. Ono, K. Watanabe, K. Nakao, Y. Konishi, R. Kishi and K. Kaya, Photoelectron spectroscopy of $(C_6F_6)_n^-$ and $(Au–C_6F_6)^-$ clusters 214 (1993) 22
Nakajima, T., see H. Sekiya 215 (1993) 499
Nakamatsu, H., see J. Onoe 217 (1994) 61
Nakamichi, Y., see Y. Mori 211 (1993) 421
Nakamura, Y., see M. Wakasa 215 (1993) 631
Nakamura, Y., M. Igarashi, Y. Sakaguchi and H. Hayashi, Effects of high magnetic fields on the dynamic behavior of radical pairs generated in micellar solutions 217 (1994) 387
Nakao, K., see A. Nakajima 214 (1993) 22
Nakao, Y., see K. Kikuchi 216 (1993) 67
Nakata, S., see K. Yoshikawa 211 (1993) 211
Nakayama, T., C. Honma, S. Miki and K. Hamanoue, Intra- and inter-molecular hydrogen-atom abstraction of photoexcited 1,4-dimethylanthraquinone 213 (1993) 581

Nakayama, T., T. Takahashi, K. Ibuki and K. Hamanoue, Intracomplex electron transfer upon direct excitation of a ground-state complex of benzophenone with 2,5-dimethyl-2,4-hexadiene 215 (1993) 622
Nakayama, T., S. Miki, F.M. Abdel-Latif, K. Ibuki and K. Hamanoue, Spectroscopic study of the formation and decay of intermediates for the novel photochemistry of sterically strained [6]-1,4-cyclophaneanthraquinone 220 (1994) 219
Nanayakkara, A., see J. Cioslowski 219 (1994) 151
Nandi, P.K., see T. Kar 220 (1994) 133
Nath, D., see N. Sarkar 218 (1994) 492
Nath, S., see P.K. Chattaraj 212 (1993) 223; 217 (1994) 342
Naujok, R.R., see D.A. Higgins 213 (1993) 485
Nedachi, K., see K. Mukai 214 (1993) 559
Neeb, M., J.-E. Rubensson, M. Biermann, W. Eberhardt, K.J. Randall, J. Feldhaus, A.L.D. Kilcoyne, A.M. Bradshaw, Z. Xu, P.D. Johnson and Y. Ma, Effects of time evolution of coherently excited vibrations in molecular core–hole decay spectra of O_2 212 (1993) 205
Negri, F., G. Orlandi, F. Zerbetto, G. Ruani, A. Zakhidov, C. Taliani, K. Kinuchi and Y. Achiba, Scattering of the vibrational frequencies of $^{13}C_x{}^{12}C_{60-x}$. A Raman spectroscopy and quantum chemical study 211 (1993) 353
Negri, F., see J.R. Morton 218 (1994) 467
Nelson, K.A., see R. Inaba 211 (1993) 183
Nemes, L., R.S. Ram, P.F. Bernath, F.A. Tinker, M.C. Zumwalt, L.D. Lamb and D.R. Huffman, Gas-phase infrared emission spectra of C_{60} and C_{70}. Temperature-dependent studies 218 (1994) 295
Nemeth, G.I., H.L. Selzle and E.W. Schlag, Magnetic ZEKE experiments with mass analysis 215 (1993) 151
Nerushev, O.A., see V.A. Maltsev 212 (1993) 480
Neugebauer, S.M. and D.S. Tinti, Deuterium isotope effects on the zero-field splittings of the lowest triplet state of benzaldehyde derivatives 211 (1993) 555
Neumann, B., Zs. Nagy-Ungvarai and S.C. Müller, Interaction between silica gel matrices and the Belousov–Zhabotinsky reaction 211 (1993) 36
Neumann, M., see Ch. Zubrägel 219 (1994) 127
Neumark, D.M., see D.J. Leahy 216 (1993) 503
Neusser, H.J., see H. Krause 213 (1993) 603
Ng, C.Y., see Z.-X. Ma 213 (1993) 250
Ng, S.C., see I. Novak 215 (1993) 561
Nguyen, M.T., L. Landuyt and L.G. Vanquickenborne, 1,3-hydrogen shift in phosphapropenes. Suprafacial sigmatropic rearrangements 212 (1993) 543
Nguyen Vien, G., N. Rougeau and C. Kubach, H-atom exchange in low energy $IH(v=0)+I$ collisions. Effect of the potential energy surface 215 (1993) 35
Nicholson, D., see A. Boutin 219 (1994) 484
Nickel, B., see M.T. Wick 215 (1993) 243
Nicolaides, C.A., T. Mercouris and I.D. Petsalakis, Above and below threshold multiphoton dissociation of volcanic ground states. Application to BeH 212 (1993) 685
Nicolaisen, H.-W., see H. Harder 214 (1993) 265
Nicula, S. and G. Bodenhausen, Triple-quantum NMR by selective triple resonance 219 (1994) 291
Niedner-Schatteburg, G., see C. Berg 216 (1993) 465
Nielsen, O.J. and J. Sehested, Upper limits for the rate constants of the reactions of CF_3O_2 and CF_3O radicals with ozone at 295 K 213 (1993) 433

Nielsen, O.J., see J. Sehested 213 (1993) 457
Nielsen, O.J., see E.L. Thomsen 215 (1993) 257
Nielsen, O.J., see C. Kelly 218 (1994) 29
Nielsen, O.J., see T.J. Wallington 218 (1994) 34
Nielsen, O.J., see T. Ellermann 218 (1994) 287
Nieminen, J. and E. Kauppi, Potential energy surface and vibrational analysis along the stretching vibrations of the $ArHAr^+$ ion 217 (1994) 31
Nienhaus, G.U., see K. Chu 216 (1993) 275
Nikiforov, A.P. and V.E. Skurat, Kinetics of polyimide etching by supersonic beams consisting of atomic and molecular oxygen mixtures 212 (1993) 43
Nikl, M., E. Mihokova, K. Nitsch, K. Polak, M. Rodova, M. Dusek, G.P. Pazzi, P. Fabeni, L. Salvini and M. Gurioli, Photoluminescence and decay kinetics of $CsPbCl_3$ single crystals 220 (1994) 14
Ning, C. and J. Pfab, Surface photochemistry of molecular solids. Dissociative desorption of NO from ClNO by pulsed 193 nm laser radiation 216 (1993) 87
Nishijima, M., see T. Takaoka 215 (1993) 523
Nishikawa, K., see H. Nagao 215 (1993) 5
Nishimura, M., see S. Murata 219 (1994) 200
Nishimura, Y., see M. Mimuro 213 (1993) 576
Nishimura, Y., see H. Sekiya 215 (1993) 499, 641
Nishina, Y., see Y. Saito 212 (1993) 379
Nishina, Y., see X.-D. Wang 216 (1993) 409
Nisoli, M., V. Pruneri, S. De Silvestri, V. Magni, A.M. Gallazzi, C. Romanoni, G. Zerbi and G. Zotti, Ultrafast non-linear optical response and acoustic phonon generation in poly(alkoxy-thiophene) film with regioregular structure 220 (1994) 64
Nitsch, K., see M. Nikl 220 (1994) 14
Nitta, A., see S. Yamamoto 215 (1993) 323
Nitta, T., see Y. Nagano 217 (1994) 186
Nizkorodov, S.A., V.I. Makarov, I.V. Khmelinskii, S.A. Kotschubei and K.A. Amosov, Time-resolved fluorescence of NO_2 in a magnetic field 215 (1993) 662
Nobusada, K., K. Sakimoto and K. Onda, Quantum mechanical close coupling calculations of collision-induced dissociation in $He+H_2$. A discretized continuum model 216 (1993) 613
Noda, C., see X. Yang 214 (1993) 536
Nogueira, M.M., see F.J. Aoiz 211 (1993) 72
Nordh, U., see N.P. Benetis 218 (1994) 551
Nordholm, S., see L. Ming 211 (1993) 189
Nordio, P.L., see A. Ferrarini 214 (1993) 409
Norris, J.R., see J. Tang 219 (1994) 283
Nørskov, J.K., see O.B. Christensen 214 (1993) 443
Novak, I., S.C. Ng and A.W. Potts, The photoelectron spectrum of a chiral molecule CHFClBr 215 (1993) 561
Novaro, O., see R. Santamaria 218 (1994) 395
Novopashin, S.A., see V.A. Maltsev 212 (1993) 480
Nunes, L.A., see S.J.L. Ribeiro 220 (1994) 214
Núñez, J., see V.G. Baonza 216 (1993) 579
Nunzi, J.-M., N. Pfeffer, F. Charra and D. Fichou, Picosecond photoinduced dichroism in sexithiophene thin films 215 (1993) 114

Nunzi, J.-M., F. Charra, C. Fiorini and J. Zyss, Transient optically induced non-centrosymmetry in a solution of octupolar molecules 219 (1994) 349
Nurgaleev, I., see S. Hess 216 (1993) 247
Nyman, G., see L. Ming 211 (1993) 189

Obi, K., see K. Saito 215 (1993) 193
Obi, K., see A. Kawai 215 (1993) 203
Obi, K., see H. Ikeura 217 (1994) 131
Odom, G.K., see K. Raghavachari 214 (1993) 357
Odom, G.K., see D.L. Strout 214 (1993) 576
Ogata, H., see E. Frankevich 214 (1993) 39
Ohashi, M., Z. Song, Y. Matsumi and M. Kawasaki, Primary processes and energy disposal in the reaction of S(^{1}D) atoms with thiirane 220 (1994) 7
Ohki, H., see N. Kimura 220 (1994) 40
Ohkubo, T., see H. Mukaihata 211 (1993) 140
Öhrn, Y., see B. Champagne 217 (1994) 551
Öhrn, Y., see R. Longo 220 (1994) 305
Ohshima, Y. and Y. Endo, Fourier-transform microwave spectroscopy of $^{24}Mg^{35}Cl$ generated by laser ablation 213 (1993) 95
Ohta, K. and T. Shima, An ab initio MO study of butalene 217 (1994) 7
Okada, T., see A. Osuka 215 (1993) 179
Okahara, K., see K. Yoshizawa 213 (1993) 498
Okahara, K., K. Tanaka, H. Aoki, T. Sato and T. Yamabe, Band structures of carbon nanotubes with bond-alternation patterns 219 (1994) 462
Okazaki, M., see Y. Fujiwara 213 (1993) 89
Okazaki, N., see Y. Mori 211 (1993) 421
Okazaki, N., see T. Sekiguchi 219 (1994) 81
Okruss, M., B. Rosenow and A. Hese, Electric properties of organic molecules. The ground and excited vibronic state dipole moments of 1-fluoronaphthalene 220 (1994) 286
Okuda, M., see Y. Saito 212 (1993) 379
Okumura, M., W. Mori and K. Yamaguchi, A MO-theoretical calculation of the antiferromagnetism in the γ-phase of *p*-nitrophenyl nitronyl nitroxide 219 (1994) 36
Oldfield, E., see J.D. Augspurger 213 (1993) 211
Olegário, R.M., see A.D. Buckingham 212 (1993) 253
Oliveira, P.W., see P. Judeinstein 220 (1994) 35
Olivucci, M., see M.J. Bearpark 217 (1994) 513
Olsen, J., see D. Sundholm 217 (1994) 451
Olsson, L. and D. Cremer, Evidence for the existence of silylium cations in condensed phases 215 (1993) 433
O'Malley, P.J., H. Soscun and S.J. Collins, The "true" minimum energy structure of $H_3SiOHAlH_3$. Implications for conformational preferences of bridged hydroxyl groups in zeolites 217 (1994) 293
Onda, K., see K. Nobusada 216 (1993) 613
Ondřejček, M., W. Stenzel, H. Conrad, V. Cháb, Z. Chvoj, W. Engel and A.M. Bradshaw, Surface diffusion of K on Pd{111} studied by photoemission electron microscopy 215 (1993) 528
Ondrias, M.R., see M.C. Schneebeck 215 (1993) 251
O'Neil, R.H., see J.Z. Zhang 218 (1994) 479
Ong, S., see X. Zhao 214 (1993) 203
Onida, G., W. Andreoni, J. Kohanoff and M. Parrinello, Ab initio molecular dynamics of C_{70}. Intramolecular vibrations and zero-point motion effects 219 (1994) 1
Onishi, M., see H. Miki 218 (1994) 563
Ono, F., see A. Nakajima 214 (1993) 22
Ono, H., see K. Misawa 220 (1994) 251

Onoe, J., R. Sekine, K. Takeuchi, H. Nakamatsu, T. Mukoyama and H. Adachi, Atomic-number dependence of relativistic effects on chemical bonding using the non-relativistic and relativistic discrete-variational Xα methods 217 (1994) 61
Onori, G., see M. D'Angelo 220 (1994) 59
Onuchic, J.N., see S.S. Skourtis 211 (1993) 282
Ookubo, N., see M. Tomonari 215 (1993) 45
Orendi, H., see Z. Sekkat 220 (1994) 497
Orlandi, G., see F. Negri 211 (1993) 353
Orlik, W., see Th. Reiners 215 (1993) 357
Orr-Ewing, A.J., see N.E. Shafer 212 (1993) 155
Orr-Ewing, A.J., see W.R. Simpson 212 (1993) 163
Ortí, E., see M.C. Piqueras 213 (1993) 509
Ortiz, J.V., Electron propagator theory of BS_2 and BS_2^- electronic structure 214 (1993) 467
Ortiz, J.V., Electron propagator calculations on the electron affinity of C_5 216 (1993) 319
Orts, J.M., see S. Remita 218 (1994) 115
Osborn, D.L., see D.J. Leahy 216 (1993) 503
Osuka, A., R.-P. Zhang, K. Maruyama, N. Mataga, Y. Tanaka and T. Okada, Determination of rates of hole transfer from free-base porphyrin to zinc porphyrin across aromatic spacers 215 (1993) 179
Oswald, M., see P. Botschwina 215 (1993) 681
Oswald, R., see P. Botschwina 215 (1993) 681
Ottinger, Ch. and A.F. Vilesov, LIF detection of the A′ $^5\Sigma_g^+$ state of N_2 in a beam and lifetime of the C″ $^5\Pi_u$ state 211 (1993) 175
Oujja, M., see M. Castillejo 214 (1993) 227
Oumi, M., see M. Head-Gordon 219 (1994) 21
Over, H., see H. Bludau 219 (1994) 452
Oyler, N.A. and L. Adamowicz, Theoretical ab initio calculations of the electron affinity of thymine 219 (1994) 223
Ozaki, Y., see H. Uehara 213 (1993) 101; 214 (1993) 527; 215 (1993) 505

Pacchioni, G., see L.G.M. Pettersson 219 (1994) 107
Packwood, T.J. and M. Page, Theoretical characterization of the potential energy surface for the reaction of SiH_3 with NO_2. Nitrosilane, silylnitrite, and the nitro–nitrite rearrangement 216 (1993) 180
Paddon-Row, M.N., see N.L. Ma 213 (1993) 189
Page, M., see T.J. Packwood 216 (1993) 180
Pagsberg, P., see T. Ellermann 218 (1994) 287
Painelli, A., see A. Fortunelli 214 (1993) 402
Paizs, B. and I. Mayer, Coupled perturbed Hartree–Fock equations. An alternative derivation and generalization to non-orthogonal orbitals 220 (1994) 97
Pal, S., see K.B. Ghose 211 (1993) 15
Palewska, K., see J. Sworakowski 220 (1994) 197
Palke, W.E., see G. von Helden 212 (1993) 247
Palstra, T.T.M., see R.C. Haddon 218 (1994) 100
Pan, X. and R.A. MacPhail, A Raman study of cyclopentane-d_9 pseudorotation dynamics as a function of pressure 212 (1993) 64
Panas, I., Structures of some hydrogen-bonded molecular clusters from ab initio hard-spheres electrostatics 216 (1993) 173
Pandey, G.C., see R.V. Jasra 211 (1993) 214
Pandey, R., M. Coolidge and W. Lauderdale, NLO properties of $Si(OH)_4$ and $Ge(OH)_4$ clusters 220 (1994) 337
Papakondylis, A. and A. Mavridis, Electronic and geometrical structure of the NF_2 radical 216 (1993) 167
Pappalardo, R.R., M. Reguero, M.A. Robb and M. Frish, Calculation of solvatochromic shifts using MC-SCF theory. The n–π^* transition of acetone 212 (1993) 12
Parak, F., see V.I. Goldanskii 219 (1994) 379
Parisse, C., see J. Brion 213 (1993) 610
Park, C.-H., B.O. Wells, J. DiCarlo, Z.-X. Shen, J.R. Salem, D.S. Bethune, C.S. Yannoni, R.D. Johnson, M.S. De Vries, C. Booth, F. Bridges and P. Pianetta, Structural information on Y ions in C_{82} from EXAFS experiments 213 (1993) 196
Park, I.J. and S.I. Woo, Computer simulation of spatial coupling in chemical oscillations of CO oxidation on two Pd(110) single crystals 212 (1993) 505
Park, J. and J.F. Hershberger, Kinetics of NCO + hydrocarbon reactions 218 (1994) 537
Park, J.K. and H. Sun, Dipole moment functions of NH and NH^+ by ab initio effective valence shell Hamiltonian 211 (1993) 618
Parker, D.H., see G. van den Hoek 215 (1993) 461
Parker, D.H., see G. Meijer 217 (1994) 112
Parmigiani, F. and L. Sangaletti, Electronic correlation effects in the Ni 3s and Co 3s X-ray photoelectron spectra of NiO, CoO, K_2NiF_4 and K_2CoF_4 213 (1993) 613
Parmigiani, F., see L.E. Depero 214 (1993) 208
Parnis, J.M., R.D. Lafleur and D.M. Rayner, Alkane reactivity with Zr atoms and neutral diatomic ZrO in the gas phase 218 (1994) 544
Parrinello, M., see G. Onida 219 (1994) 1
Partridge, H., see C.W. Bauschlicher Jr. 211 (1993) 312; 215 (1993) 451; 216 (1993) 341
Pasinszki, T., T. Veszprémi and M. Fehér, The structure of beryllium pseudohalides 215 (1993) 395
Pasternack, L., see R.E. McClean 215 (1993) 209
Patterson, C.H., A novel method for computing bond–bond interactions of large systems 213 (1993) 59
Payne, M.C., see D.M. Bird 212 (1993) 518

Payne, M.C., see I. Štich 212 (1993) 617
Paz, J.L., M. García-Sucre, E. Squitieri and V. Mujica, The effect of intramolecular coupling on the optical susceptibilities of a two-level molecule 217 (1994) 333
Pazzi, G.P., see M. Nikl 220 (1994) 14
Pédrini, C., D. Bouttet, C. Dujardin, B. Moine and H. Bill, Spectroscopic studies of the f↔d ultraviolet transitions of Pr^{3+} in alkaline earth fluorides 220 (1994) 433
Peel, J.B., Configuration interaction calculations of the structure and energetics of the high symmetry isomers of the O_4^+ cation 218 (1994) 367
Pei, C., see K. Chen 217 (1994) 471
Pélissier, M., see T. Leininger 220 (1994) 345
Pellarin, M., B. Baguenard, J.L. Vialle, J. Lermé, M. Broyer, J. Miller and A. Perez, Evidence for icosahedral atomic shell structure in nickel and cobalt clusters. Comparison with iron clusters 217 (1994) 349
Pellenq, R.J.-M., see A. Boutin 219 (1994) 484
Pemble, M.E., see P. Bond 211 (1993) 649
Pépin, C., see T.-H. Tran-Thi 213 (1993) 139
Perchard, J.P., see S. Coussan 217 (1994) 123
Perel, A.S., see R.C. Haddon 218 (1994) 100
Peremans, A. and A. Tadjeddine, Spectroscopic investigation of Pt–methanol interface in perchloric acid medium by sum-frequency generation 220 (1994) 481
Perera, L., see L.S. Sremaniak 218 (1994) 377
Perera, S.A. and R.J. Bartlett, Relativistic effects at the correlated level. An application to interhalogens 216 (1993) 606
Perez, A., see M. Pellarin 217 (1994) 349
Pérez-Jordá, J.M., see M. Hồ 219 (1994) 15
Permogorov, D., see A. Charvát 214 (1993) 495
Persson, A., see P. Erman 215 (1993) 173
Petek, H., see P.B. Bisht 213 (1993) 75
Petek, H., see H. Sekiya 215 (1993) 641
Petelenz, P., Nonlocal polarizabilities in excited states of polyacene crystals 215 (1993) 607
Petersen, B.L., L.J. Terminello, J.J. Barton and D.A. Shirley, Photoelectron holography of Pt(111) at 351 eV 213 (1993) 412
Petersen, B.L., L.J. Terminello, J.J. Barton and D.A. Shirley, Multiple-wavenumber photoelectron holography of Pt(111) 220 (1994) 46
Petrella, G. and L. Cassidei, Atom scattering from disordered surfaces. Theoretical study on the validity of the cross section overlap hypothesis: the case of vacancies on Pt(111) 212 (1993) 512
Petricek, V., see J.L. de Boer 219 (1994) 469
Petrillo, C.J., see X. Yang 214 (1993) 536
Petsalakis, I.D., see C.A. Nicolaides 212 (1993) 685
Pettersson, L.G.M. and G. Pacchioni, The electronic structure of an oxygen defect in NiO(100) 219 (1994) 107
Petteway, J.C., see D.A. Baugh 219 (1994) 207
Peyerimhoff, S.D., see M. Carnell 212 (1993) 654
Peyerimhoff, S.D., see S. Grimme 213 (1993) 32
Pfab, J., see C. Ning 216 (1993) 87
Pfeffer, N., see J.-M. Nunzi 215 (1993) 114
Philipp, R., see K. Chu 216 (1993) 275

Pianetta, P., see C.-H. Park 213 (1993) 196
Pick, Š., see P. Mikušík 215 (1993) 319
Pierloot, K., E. Tsokos and B.O. Roos, 3p–3d intershell correlation effects in transition metal ions 214 (1993) 583
Pilloud, D., see E. Vauthey 215 (1993) 264
Pinegar, J.C., J.D. Langenberg and M.D. Morse, Spectroscopy of jet-cooled Ag_2Au 212 (1993) 458
Pines, A., see R.G. Larsen 214 (1993) 220
Pipes, L.C., see D.A. Baugh 219 (1994) 207
Piqueras, M.C., R. Crespo, E. Ortí and F. Tomás, AM1 prediction of the equilibrium geometry of Si_{60} 213 (1993) 509
Pittner, J., see V. Bonačić-Koutecký 213 (1993) 522
Pizio, O. and L. Pusztai, Triplet correlations in the molten phase of Ag_2Se superionic conductor 214 (1993) 125
Plakhotnik, T., see F. Güttler 217 (1994) 393
Planeix, J.M., see P.M. Ajayan 215 (1993) 509
Plitt, H.S., V. Balaji and J. Michl, Localization of singlet excitation in short silicon chains, Si_2Me_6 to Si_6Me_{14} 213 (1993) 158
Poblet, J.M., see C. Sousa 215 (1993) 97
Pogrebnya, S.K. and D.C. Clary, Coupled states calculations on vibrational relaxation of N_2^+ in collisions with He 219 (1994) 366
Polak, K., see M. Nikl 220 (1994) 14
Polanz, O., see M. Saarinen 219 (1994) 181
Polezzo, S., see V. Bonačić-Koutecký 213 (1993) 522
Poliakoff, M., see A.I. Cooper 212 (1993) 611
Politzer, P. and J.M. Seminario, Computational study of the structure of dinitraminic acid, $HN(NO_2)_2$, and the energetics of some possible decomposition steps 216 (1993) 348
Poljanskii, S.V., see A.V. Larin 213 (1993) 619
Poll, J.D., see C.G. Joslin 211 (1993) 587; 213 (1993) 377; 215 (1993) 144
Poll, J.D., see W. Głaz 218 (1994) 183
Poluektov, O.G., see M. Matsushita 214 (1993) 349
Poluektov, O.G., see D.S. Tipikin 215 (1993) 199
Polzonetti, G., M.V. Russo, A. Furlani and G. Infante, Cr metallization of polyphenylacetylene thin film investigated by XPS 214 (1993) 333
Pommier, J., see R. Abouaf 213 (1993) 503
Ponterini, G., see M. Caselli 216 (1993) 41
Pople, J.A., see L.A. Curtiss 214 (1993) 183
Pople, J.A., see K. Raghavachari 214 (1993) 357; 220 (1994) 385
Pople, J.A., see P.M.W. Gill 217 (1994) 65
Pople, J.A., see B.G. Johnson 218 (1994) 595; 220 (1994) 377
Popov, S.V., see A.R. Bungay 217 (1994) 249
Popovic, Z.D. and S. Mesbah, Slope to intercept ratio of low-field photogeneration efficiency in β-metal-free phthalocyanine 215 (1993) 636
Port, H., see J. Walz 213 (1993) 321
Porter, C.F., see N. Tamai 211 (1993) 364
Potts, A.W., see I. Novak 215 (1993) 561
Povill, À., J. Rubio, R. Caballol and J.P. Malrieu, The full-CI energy of the NH_3 molecule in a DZP basis set 218 (1994) 283

Powell, B.M., see J.S. Tse 215 (1993) 383
Powis, I., Continuum MS-Xα calculations for core and outer valence shell photoionization of PF_3 215 (1993) 269
Prasad, B.V., see G. Subramanian 217 (1994) 296
Pratt, S.T., see E.F. McCormack 211 (1993) 147
Pravilov, A.M., see A.A. Matveev 217 (1994) 582
Preston, K.F., see J.R. Morton 218 (1994) 467
Preuss, H., see E. Czuchaj 212 (1993) 534; 218 (1994) 454
Price, S.D., M. Manning and S.R. Leone, Collision-induced neutral loss reactions of molecular dications 214 (1993) 553
Prieto, M., see A. Aguilar 220 (1994) 267
Prince, K.C., see C. Comicioli 214 (1993) 438
Pritchard, H.P., see J.F. Ying 212 (1993) 289
Prochorow, J., see N. Fukazawa 220 (1994) 461
Protsykevytch, I.A., see Yu.V. Kalyuzhnyi 215 (1993) 1
Pruneri, V., see M. Nisoli 220 (1994) 64
Pullerits, T., see S. Hess 216 (1993) 247
Purnell, J., see S.F. Cartier 220 (1994) 23
Puschmann, A., see G. Remmers 214 (1993) 241
Pusztai, L., see O. Pizio 214 (1993) 125
Pyne, C.H., see A. Carrington 212 (1993) 473
Pyper, N.C., The relative stability of the six- and eight-fold co-ordinated structures of cesium chloride 220 (1994) 70
Pyykkö, P., J. Li and N. Runeberg, Predicted ligand dependence of the Au(I)...Au(I) attraction in $(XAuPH_3)_2$ 218 (1994) 133

Qian, C.X.W., see Y. Wang 219 (1994) 389
Qin, S., W.-M. You and Z.-B. Su, Theoretical approach to EPR spectrum of C_{60}^- in molecular sieve 13X 213 (1993) 373
Quack, M., see D. Luckhaus 212 (1993) 434
Quack, M., see H. Gross 213 (1993) 122
Quack, M., see Y. He 215 (1993) 228
Que, W., see D.F. Agterberg 213 (1993) 207
Queffelec, J.-L., see I.R. Sims 211 (1993) 461
Quintella, C.M., A.J. McCaffery and M.D. Zidan, Direct observation of the kinetics and dynamics of molecular desorption from liquid surfaces 214 (1993) 563

Rabinowitz, M., Phenomenological theory for short coherence length superconductivity 216 (1993) 571
Rabinowitz, M. and T. McMullen, General model of pressure-induced transition temperature increase with focus on the Hg–Ba–Ca–Cu–O system 218 (1994) 437
Rabus, H., see D. Arvanitis 211 (1993) 53
Rachinsky, A.G. and V.F. Razumov, Photochemistry of amorphous 1,2-di-(α-naphthyl)ethylene 219 (1994) 421
Rachlew-Källne, E., see P. Erman 215 (1993) 173
Racine, S., see S. Coussan 217 (1994) 123
Radenkovic, B., see B.R. Jovanic 216 (1993) 47
Radom, L., see A.P. Scott 212 (1993) 705
Raghavachari, K., see L.A. Curtiss 214 (1993) 183
Raghavachari, K., D.L. Strout, G.K. Odom, G.E. Scuseria, J.A. Pople, B.G. Johnson and P.M.W. Gill, Isomers of C_{20}. Dramatic effect of gradient corrections in density functional theory 214 (1993) 357
Raghavachari, K., B. Zhang, J.A. Pople, B.G. Johnson and P.M.W. Gill, Isomers of C_{24}. Density functional studies including gradient corrections 220 (1994) 385
Rai, S.N., see H.-P. Liebermann 214 (1993) 381
Rajagopalan, V., see P.S. Goyal 211 (1993) 559
Rajgara, F.A., see G.R. Kumar 217 (1994) 626
Ram, R.S., see L. Nemes 218 (1994) 295
Ramachandran, B., see X. Wu 214 (1993) 118
Ramamoorthy, A., see T. Fujiwara 212 (1993) 81
Rama Rao, K.V.S., see Awadhesh Kumar 212 (1993) 103
Rama Rao, K.V.S., see P.K. Chowdhury 218 (1994) 60
Ramasesha, S.K., A.K. Singh, R. Seshadri, A.K. Sood and C.N.R. Rao, Orientational ordering in C_{70}. Evidence for three distinct phase transitions 220 (1994) 203
Ramiro Diaz, B., P. Wahnon and V. Sidis, A calculated $(KrO_2)^+$ ground-state potential energy surface 212 (1993) 218
Randall, K.J., see M. Neeb 212 (1993) 205
Randić, M., Novel molecular descriptor for structure–property studies 211 (1993) 478
Ranz, R., see Y. He 215 (1993) 228
Rao, A.M., see P. Zhou 211 (1993) 337
Rao, C.N.R., see A. Chakrabarti 215 (1993) 591
Rao, C.N.R., see S.P. Ananthavel 217 (1994) 101
Rao, C.N.R., see D.V.S. Muthu 217 (1994) 146
Rao, C.N.R., see S.K. Ramasesha 220 (1994) 203
Rao, K.V., see R.V. Jasra 211 (1993) 214
Rashev, S., What is the mechanism of vibrational redistribution around E_{2g} states in S_1 benzene, Coriolis or anharmonic? 211 (1993) 613
Rashev, S., A theoretical study of internal conversion in benzene 217 (1994) 69
Rassat, A., see B. Keita 215 (1993) 125
Rastomjee, C.S., see B. Rausenberger 215 (1993) 109
Rausenberger, B., W. Swiech, C.S. Rastomjee, M. Mundschau, W. Engel, E. Zeitler and A.M. Bradshaw, Imaging reaction–diffusion fronts with low-energy electron microscopy 215 (1993) 109
Ravichandran, K., R. Williams and T.R. Fletcher, Atmospheric reactions of vibrationally excited greenhouse gases: $SH + N_2O(n, 0, 0)$ 217 (1994) 375
Raviprasad, G.V. and A.M. Jayannavar, Friction dependence of reaction rates in simple barrierless reactions 220 (1994) 353

Ray, D., see R. Knochenmuss 215 (1993) 188
Rayez, J.C., see L. Bonnet 216 (1993) 11
Rayner, D.M., see K. Athanassenas 213 (1993) 105
Rayner, D.M., see J.M. Parnis 218 (1994) 544
Rayner, S.P., see M. Baba 220 (1994) 411
Raynes, W.T., see M. Grayson 214 (1993) 473; 218 (1994) 270
Raz, T., see M. Ben-Nun 220 (1994) 291
Razumov, V.F., see A.G. Rachinsky 219 (1994) 421
Rebentrost, F., see E. Czuchaj 212 (1993) 534; 218 (1994) 454
Reguero, M., see R.R. Pappalardo 212 (1993) 12
Reid, B.P., see J.L. Tomer 216 (1993) 286
Reid, K.L., Effect of intermediate state depolarization on photoelectron angular distributions from molecules following (1+1′) REMPI 215 (1993) 25
Reilly, J.P., see Z. Lin 217 (1994) 239
Reilly, P.T.A., see R. Liyanage 216 (1993) 544
Reiners, Th., W. Orlik, Ch. Ellert, M. Schmidt and H. Haberland, Temperature dependence of the Na_n^+ optical response 215 (1993) 357
Reininger, R., see M. Chergui 216 (1993) 34
Reininger, R., see A. Al-Omari 220 (1994) 437
Reis e Sousa, A.T., E.M.S. Castanheira, J.M.G. Martinho, S. Saghbini, F. Baros, J.C. André and M.A. Winnik, Influence of pressure on cyclization of a polystyrene chain. Time-resolved fluorescence measurements 213 (1993) 333
Reisfeld, R., see R. Gvishi 212 (1993) 463; 213 (1993) 338
Reisfeld, R., see D. Shamrakov 213 (1993) 47
Remita, S., J.M. Orts, J.M. Feliu, M. Mostafavi and M.O. Delcourt, STM identification of silver oligomer clusters prepared by radiolysis in aqueous solution 218 (1994) 115
Remmers, G., M. Domke, A. Puschmann, T. Mandel, G. Kaindl, E. Hudson and D.A. Shirley, High-resolution inner-shell photoionization of NO 214 (1993) 241
Rempel, U., see E. Laitinen 218 (1994) 73
Renge, I., see R.B. Altmann 216 (1993) 281
Renn, A., see M. Croci 212 (1993) 71
Renn, A., see F. Güttler 217 (1994) 393
Rentsch, S., see D.V. Lap 211 (1993) 135
Rerat, M., see A. Lichanot 211 (1993) 249
Reynhardt, E.C. and A. Wozniak-Braszak, Polymorphism and molecular motions in *n*-nonylammonium chloride 215 (1993) 493
Ribeiro, S.J.L., R.E.O. Diniz, Y. Messaddeq, L.A. Nunes and M.A. Aegerter, Eu^{3+} and Gd^{3+} spectroscopy in fluoroindate glasses 220 (1994) 214
Ribeiro-Claro, P.J.A., see R.D. Gordon 211 (1993) 392
Ricciardi, G., F. Lelj and F. Bonosi, Synthesis and physico-chemical properties of the bis(2,3,7,8,12,13,17,18-octakis-(octhylthio)-5,10,15,20-tetraazaporphyrinato)-lutetium(III) complex 215 (1993) 541
Rice, B.M., H.E. Cartland and C.F. Chabalowski, Ab initio potential energy surface for the H+OCS reaction 211 (1993) 283
Richardson, F.S., see J.P. Bolender 213 (1993) 131
Richert, R., Origin of dispersion in dipolar relaxations of glasses 216 (1993) 223
Richmond, G.L., see K.A. Friedrich 213 (1993) 491

Richmond, G.L., see P.R. Fischer 218 (1994) 200
Rico, R.J. and M. Head-Gordon, Single-reference theories of molecular excited states with single and double substitutions 213 (1993) 224
Rico, R.J., T.J. Lee and M. Head-Gordon, The origin of differences between coupled cluster theory and quadratic configuration interaction for excited states 218 (1994) 139
Rico, R.J., see M. Head-Gordon 219 (1994) 21
Ridley, T., see M.S.N. Al-Kahali 220 (1994) 225
Rieder, K.H., see R. Koch 220 (1994) 172
Riehl, J.-F., see T. Leininger 220 (1994) 345
Riehl, J.P., see S.C.J. Meskers 216 (1993) 241
Riehl, K., see J. Holtgrave 215 (1993) 548
Rieker, A., see G.G. Lazarev 212 (1993) 319
Riesen, H. and E. Krausz, Stark-swept transient hole burning and resonant luminescence line narrowing in $[Zn(2,2'\text{-bipyridine})_3](ClO_4)_2$:Ru(II) 212 (1993) 347
Riesen, H. and E. Krausz, Orientational dependences of the Zeeman effect in the lowest-excited states of $[Zn(bpy)_3](ClO_4)_2$:Ru(II) and $[Ru(bpy)_3](PF_6)_2$ 217 (1994) 613
Riesen, H., E. Krausz and L. Dubicki, Probing the distribution of low symmetry fields by the magnetic field effect on a persistent spectral hole in the R_1 line of chromium(III)-tris(2,2'-bipyridine) in glycerol 218 (1994) 579
Righini, R., see R. Torre 212 (1993) 90
Rinnemo, M., M. Fassihi and B. Kasemo, The critical condition for catalytic ignition. H_2/O_2 on Pt 211 (1993) 60
Roark, S.E. and K.L. Rowlen, Atomic force microscopy of thin Ag films. Relationship between morphology and optical properties 212 (1993) 50
Robb, M.A., see R.R. Pappalardo 212 (1993) 12
Robb, M.A., see M.J. Bearpark 217 (1994) 513
Robert, J.B., see D. Canet 212 (1993) 483
Roberti, T.W., see J.Z. Zhang 218 (1994) 479
Robinson, K.M., see A.A. Kornyshev 219 (1994) 132
Robl, R., see P. Scheier 220 (1994) 141
Robyr, P., see M. Tomaselli 214 (1993) 1
Rocca, D., see A. De Santis 213 (1993) 239
Roco, J.M.M., A. Medina, A. Calvo Hernández and S. Velasco, Theoretical far-infrared spectra of CO in Ar gas 216 (1993) 593
Rodgers, A.S., Conservation of angular momentum in RRKM theory. A three-dimensional model for nonlinear molecules 219 (1994) 297
Rodgers, D., see A. Mank 219 (1994) 169
Rodova, M., see M. Nikl 220 (1994) 14
Rodriguez, J.A. and J. Hrbek, Synergistic interactions in three-center metal–metal bonding. Cu–Zn on Ru(0001) 220 (1994) 486
Rogemond, F., H. Chermette and D.R. Salahub, Analysis and assignment of the optical absorption transitions in $CuCl_2$ with Gaussian density functional calculations 219 (1994) 228
Rohlfing, C.M., see C.C. Henderson 213 (1993) 383
Rohmund, F., see M. Ehbrecht 214 (1993) 34
Rohrbacher, A., see M. Fehér 211 (1993) 171
Roitzsch, R., see J. Ackermann 214 (1993) 109
Romanoni, C., see M. Nisoli 220 (1994) 64

Ronfard-Haret, J.C., see S. Bachir 213 (1993) 54
Roos, B.O., see L. Serrano-Andrés 211 (1993) 125
Roos, B.O., see K. Pierloot 214 (1993) 583
Rösch, N., see S. Krüger 216 (1993) 435
Rosei, R., see D. Alfè 211 (1993) 220
Rosei, R., see C. Comicioli 214 (1993) 438
Rosenholm, J.B., see L. Laaksonen 216 (1993) 429
Rosenow, B., see M. Okruss 220 (1994) 286
Rosenwaks, S., see S. Koppe 214 (1993) 546
Roskilly, S.J., see A. Ferrarini 214 (1993) 409
Rosmus, P., see A. Spielfiedel 216 (1993) 162
Rosmus, P., see T. Schmelz 220 (1994) 117
Rosner, B., see I. Ben-Itzhak 212 (1993) 467
Ross, A.J., see R.F. Barrow 214 (1993) 293
Rossini, S., see F. Kajzar 217 (1994) 418
Rossky, P.J., see W.-S. Sheu 213 (1993) 233
Rossner, W., see E. Bayer 216 (1993) 228
Roszak, S. and K. Balasubramanian, First-principle interatomic potentials for the carbon monoxide–platinum reaction 212 (1993) 150
Roszak, S., see M. Vijayakumar 215 (1993) 87
Roszak, S., K. Balasubramanian, J.J. Kaufman and W.S. Koski, Multireference configuration interaction study of temporary anion states in haloforms 215 (1993) 427
Roth, S., see L. Akselrod 212 (1993) 384; 215 (1993) 131
Roth, S., see K. Kamarás 214 (1993) 338
Rotman, S.R., see J.A. Mares 217 (1994) 105
Rougeau, N., see G. Nguyen Vien 215 (1993) 35
Rousseau, B., see A. Boutin 218 (1994) 122
Roux, B., Non-additivity in cation–peptide interactions. A molecular dynamics and ab initio study of Na^+ in the gramicidin channel 212 (1993) 231
Rowe, B.R., see I.R. Sims 211 (1993) 461
Rowlen, K.L., see S.E. Roark 212 (1993) 50
Roy, D., see G. Nagy 214 (1993) 197
Rozas, I., see O. Mó 219 (1994) 45
Ruani, G., see F. Negri 211 (1993) 353
Rubahn, H.-G., see E.L. Knuth 213 (1993) 1
Rubensson, J.-E., see M. Neeb 212 (1993) 205
Rubio, J., S. Zurita, J.C. Barthelat and F. Illas, Electronic and geometrical structures of Pt_3 and Pt_4. An ab initio one-electron proposal 217 (1994) 283
Rubio, J., see À. Povill 218 (1994) 283
Rudich, Y., see Y. Hurwitz 215 (1993) 674
Rudolf, P., see D. Alfè 211 (1993) 220
Rudolph, H., see K. Wang 217 (1994) 490
Rühl, E., C. Heinzel and H.W. Jochims, Fluorescence of Ar(2p)-excited argon clusters 211 (1993) 403
Ruhman, S., see A. Waldman 215 (1993) 470
Rumbles, G., see I.D.W. Samuel 213 (1993) 472
Runeberg, N., see P. Pyykkö 218 (1994) 133
Rupnik, K., see U. Asaf 212 (1993) 326

Russo, M.V., see G. Polzonetti 214 (1993) 333
Russo, N., see V. Barone 212 (1993) 5
Russo, N., E. Sicilia and M. Toscano, Singlet–triplet gap in HCI halocarbene 213 (1993) 245
Ruth, A.A., see M.T. Wick 215 (1993) 243
Rutz, S., see K. Kobe 213 (1993) 554
Ruud, K., see M. Jaszunski 220 (1994) 154
Ruuskanen-Järvinen, P., see E. Laitinen 218 (1994) 73
Ryckaert, J.-P., see K.D. Hammonds 213 (1993) 27
Rzhevsky, O.S., see E.B. Gordon 217 (1994) 605

Saarinen, M., L. Halonen and O. Polanz, High-resolution photoacoustic overtone spectrum of monochloroacetylene using a titanium:sapphire ring laser spectrometer 219 (1994) 181
Saathoff, H., see Ch. Fockenberg 218 (1994) 21
Sabanayagam, C., see D.K. Kondepudi 217 (1994) 364
Sabelfeld, K.K., see B.Z. Gorbunov 215 (1993) 31
Sadlej, A.J., see P.W. Fowler 212 (1993) 659
Sáez Rábanos, V., see F.J. Aoiz 211 (1993) 72; 218 (1994) 422
Safvan, C.P., see G.R. Kumar 217 (1994) 626
Sagar, R.P., see M. Hô 219 (1994) 15
Saghbini, S., see A.T. Reis e Sousa 213 (1993) 333
Sah, C.H., see D. Babić 211 (1993) 235
Saigusa, H. and E.C. Lim, Photoionization of naphthalene clusters via excimer formation 211 (1993) 410
Sairanen, O.-P., H. Aksela, S. Aksela and M. Hotokka, Changes in molecular KLL Auger spectrum of fluorine on going from HF to LiF, NaF, and KF 215 (1993) 353
Saito, K. and K. Obi, The first observation of the $\tilde{A}\ ^1B_1$–$\tilde{X}\ ^1A_1$ transition of GeH_2 and GeD_2 radicals 215 (1993) 193
Saito, K., see K. Kikuchi 216 (1993) 67
Saito, M., see T. Yamato 219 (1994) 155
Saito, S., see M. Goto 211 (1993) 443
Saito, Y., T. Yoshikawa, M. Okuda, N. Fujimoto, S. Yamamuro, K. Wakoh, K. Sumiyama, K. Suzuki, A. Kasuya and Y. Nishina, Iron particles nesting in carbon cages grown by arc discharge 212 (1993) 379
Saito, Y., see X.-D. Wang 216 (1993) 409
Sakaguchi, Y., see M. Wakasa 215 (1993) 631
Sakaguchi, Y., see Y. Nakamura 217 (1994) 387
Sakai, S., A new mechanism of $H_2B{=}NH_2$ formation in the reaction of B_2H_6 with NH_3 217 (1994) 288
Sakimoto, K., see K. Nobusada 216 (1993) 613
Sakoda, K. and K. Kominami, Photochemical hole burning of porphin-cross-linked polymethylmethacrylate 215 (1993) 488
Sakoda, K. and K. Kominami, Photochemical hole burning of cationic porphin/saponite intercalation compounds 216 (1993) 270
Sakoda, K. and M. Maeda, Photochemical hole burning of ionic porphins and the deuterated analogues 217 (1994) 152
Saksager, O., see J. Hall 216 (1993) 413
Sakurai, T., see X.-D. Wang 216 (1993) 409
Salahub, D.R., see F. Rogemond 219 (1994) 228
Salaneck, W.R., see M. Fahlman 214 (1993) 327
Salem, J.R., see C.-H. Park 213 (1993) 196
Salikhov, K.M., see Yu.N. Molin 211 (1993) 484
Salter, R.H., see R.A. Dressler 215 (1993) 656
Salter, R.H., see T.L. Thiem 218 (1994) 309
Salvini, L., see M. Nikl 220 (1994) 14
Sammond, D.M., see T.F. Magnera 211 (1993) 378
Samoson, A., Approximate approach to DOR sideband suppression 214 (1993) 456
Samuel, I.D.W., B. Crystall, G. Rumbles, P.L. Burn, A.B. Holmes and R.H. Friend, The efficiency and time-dependence of luminescence from poly(*p*-phenylene vinylene) and derivatives 213 (1993) 472

Sangaletti, L., see F. Parmigiani 213 (1993) 613
Sannigrahi, A.B., see P.K. Chattaraj 212 (1993) 223
Sannigrahi, A.B. and F. Grein, Configuration interaction study of the potential energy surface of the three lowest singlet A′ and A″ states of HCP 214 (1993) 609
Sannigrahi, A.B., see T. Kar 220 (1994) 133
Sano, T., see K. Kobayashi 219 (1994) 53
Sánta, I., see R. Torre 212 (1993) 90
Santamaria, R., I.G. Kaplan and O. Novaro, A comparative theoretical study of stable geometries and energetic properties of small silver clusters 218 (1994) 395
Santucci, A., see M. D'Angelo 220 (1994) 59
Sapse, D., see G. Snyder 218 (1994) 372
Šarapatka, T.J., XPS-XAES study of charge transfers at $Ni/Al_2O_3/Al$ systems 212 (1993) 37
Sariciftci, N.S., see B. Kraabel 213 (1993) 389
Sarkar, N., K. Das, D. Nath and K. Bhattacharyya, Salt effect on the hydrophobic binding of *p*-toluidino naphthalene sulphonate with cyclodextrins 218 (1994) 492
Sarkisov, O.M., see A.A. Iogansen 212 (1993) 604
Sasabe, H., see H. Kandori 211 (1993) 385; 216 (1993) 126
Sastre, R., see A. Douhal 219 (1994) 91
Sato, K., see H. Umemoto 214 (1993) 271
Sato, T., see K. Yoshizawa 213 (1993) 498
Sato, T., see H. Umemoto 214 (1993) 271
Sato, T., see K. Okahara 219 (1994) 462
Satomi, R., see H. Miki 218 (1994) 563
Satpathy, S., see J. Shumway 211 (1993) 595
Sattler, K., see M. Ge 220 (1994) 192
Sauer, J. and J.-R. Hill, The acidity of surface silanol groups. A theoretical estimate based on ab initio calculations on a model surface 218 (1994) 333
Saury, A., see J.S. Baskin 214 (1993) 257
Saury, A., see R. Huang 216 (1993) 108, 115
Savin, A., see P. Fuentealba 217 (1994) 566
Sawada, M., see T. Takaoka 215 (1993) 523
Sax, A.F., see J. Kalcher 215 (1993) 601
Sax, A.F., see M.C. Ernst 216 (1993) 189
Sayós, R., see A. Aguilar 220 (1994) 267
Scarton, M.G., see M.A. Buntine 216 (1993) 471
Schallmoser, G., see N. Caspary 212 (1993) 329
Schallmoser, G., A. Thoma, B.E. Wurfel and V.E. Bondybey, Rotation of CN in solid rare gases 219 (1994) 101
Schaphorst, S.J., C.D. Caldwell, M.O. Krause and J. Jiménez-Mier, Evidence for atomic features in the decay of resonantly excited molecular oxygen 213 (1993) 315
Scheier, P., R. Robl, B. Schiestl and T.D. Märk, Electron-impact-induced production and isotope-resolved identification of C_{60}^{5+} 220 (1994) 141
Scheiner, A., see J. Baker 216 (1993) 380
Scheller, M.K. and L.S. Cederbaum, A construction principle for stable multiply charged molecular anions in the gas phase 216 (1993) 141
Scherer, P.O.J., Intramolecular charge separation in a dynamically disordered polar environment 214 (1993) 149

Schettino, V., see C. Taiti 212 (1993) 283
Schiestl, B., see P. Scheier 220 (1994) 141
Schindler, T., see C. Berg 216 (1993) 465
Schlag, E.W., see G.I. Nemeth 215 (1993) 151
Schlitter, J., Estimation of absolute and relative entropies of macromolecules using the covariance matrix 215 (1993) 617
Schlittler, R.R., see J.K. Gimzewski 213 (1993) 401; 217 (1994) 589
Schlütter, J., R. Schott and K. Kleinermanns, State selective investigation of the reactions $O(^1D)+CH_4$ $(C_2H_6)\rightarrow OH$ $(CH_2OH)+CH_3(\nu_1(v), \nu_2(v), J, K)$ using resonant multiphoton ionization detection of CH_3 213 (1993) 262
Schmelz, T. and P. Rosmus, Rovibronic energy levels of $HeHF^+$ $(X\ ^2\Pi)$ 220 (1994) 117
Schmickler, W., D. Henderson and O.R. Melroy, The dependence of the oxygen–metal distance for water adsorbed at a metal electrode 216 (1993) 424
Schmid, A., see H. Gross 213 (1993) 122
Schmid, G.M., S. Coy, R.W. Field and R.J. Silbey, Duffing's oscillator and the normal to local mode transition in AB_2 triatomic molecules 219 (1994) 331
Schmid, R., see D.V. Matyushov 220 (1994) 359
Schmidt, C., M. Warken and N.C. Handy, The Feenberg series. An alternative to the Møller–Plesset series 211 (1993) 272
Schmidt, C., see K. Dietz 220 (1994) 397
Schmidt, H., see P. Judeinstein 220 (1994) 35
Schmidt, J., see M. Matsushita 214 (1993) 349
Schmidt, J., see D.S. Tipikin 215 (1993) 199
Schmidt, K., see R. Koch 220 (1994) 172
Schmidt, M., see Th. Reiners 215 (1993) 357
Schmidt, M.W., see T.L. Windus 216 (1993) 375
Schmidt, R. and M. Bodesheim, Efficiencies of $O_2(^1\Sigma_g^+)$ and $O_2(^1\Delta_g)$ formation in the primary steps of triplet state photosensitization in solution 213 (1993) 111
Schmidt, Th., see H. van der Laan 212 (1993) 569
Schmidt-Rohr, K., see R.G. Larsen 214 (1993) 220
Schmitt, M., H. Müller and K. Kleinermanns, A study of intermolecular vibrational frequencies of phenol$\cdot(H_2O)_3$ by spectral hole burning spectroscopy 218 (1994) 246
Schneebeck, M.C., L.E. Vigil and M.R. Ondrias, Mode-selective energy localization during photoexcitation of deoxyhemoglobin and heme model complexes 215 (1993) 251
Schneider, F., see Ch. Zubrägel 219 (1994) 127
Schneider, F.W., see H. Lanig 220 (1994) 423
Schneider, S., W. Stammler, R. Bierl and W. Jäger, Ultrafast photoinduced charge separation and recombination in weakly bound complexes between oxazine dyes and N,N-dimethylaniline 219 (1994) 433
Schneider, W.F., see T.J. Wallington 213 (1993) 442; 218 (1994) 34
Schoenhofer, R., see M.E. Smith 219 (1994) 75
Schofield, S.A. and P.G. Wolynes, Rate theory and non-RRKM quantum dynamics described by local random matrix models 217 (1994) 497
Schönnenbeck, G., see J. Hohmann 217 (1994) 577
Schott, R., see J. Schlütter 213 (1993) 262
Schreiber, E., see K. Kobe 213 (1993) 554
Schreier, K.M., see D.A. Dolson 212 (1993) 118

Schriver, A., see L. Schriver-Mazzuoli 214 (1993) 519
Schriver-Mazzuoli, L., O. Abdelaoui, C. Lugez and A. Schriver, Matrix reaction of ozone with Cl_2 and Br_2. FTIR identification of BrClO and ClBrO species 214 (1993) 519
Schroeder, J., D. Schwarzer, J. Troe and P. Vöhringer, From barrier crossing to barrierless relaxation dynamics. Photoisomerization of trans-stilbene in compressed *n*-alkanols 218 (1994) 43
Schwaner, A.L., see Z.-J. Sun 219 (1994) 118
Schwarz, E., see R. Koch 220 (1994) 172
Schwarz, H., see A. Fiedler 211 (1993) 242
Schwarz, H., see N. Goldberg 213 (1993) 593
Schwarzer, D., see J. Schroeder 218 (1994) 43
Schweiger, A., see E. Hoffmann 220 (1994) 467
Schwenke, D.W., see S.L. Mielke 213 (1993) 10; 216 (1993) 441; 217 (1994) 173
Schwentner, N., see M. Chergui 219 (1994) 237
Schwerdtfeger, P., J.S. McFeaters, R.L. Stephens, M.J. Liddell, M. Dolg and B.A. Hess, Can AuF be synthesized? A theoretical study using relativistic configuration interaction and plasma modeling techniques 218 (1994) 362
Scott, A.P. and L. Radom, Reply to Comment on "Cyclopentadienylideneketene: theoretical confirmation of a key infrared band" 212 (1993) 705
Scuseria, G.E., see K. Raghavachari 214 (1993) 357
Scuseria, G.E., see D.L. Strout 214 (1993) 576
Scuseria, G.E., see W.C. Eckhoff 216 (1993) 399
Sears, V.F., see J.S. Tse 215 (1993) 383
Sebenik, C., see A.B. Finnila 219 (1994) 343
Seetula, J.A., see A.A. Iogansen 212 (1993) 604
Sehested, J., see O.J. Nielsen 213 (1993) 433
Sehested, J., O.J. Nielsen and T.J. Wallington, Absolute rate constants for the reaction of NO with a series of peroxy radicals in the gas phase at 295 K 213 (1993) 457
Sehested, J., see T.J. Wallington 218 (1994) 34
Sehested, J., see T. Ellermann 218 (1994) 287
Seifert, F., see H. Kneipp 212 (1993) 374
Sekiguchi, T., see Y. Mori 211 (1993) 421
Sekiguchi, T., see H. Ikeura 217 (1994) 131
Sekiguchi, T., Y. Mori, N. Okazaki and I. Hanazaki, Photoinduction and photoinhibition of chemical oscillations in the tris(2,2′-bipyridine)ruthenium(II)-catalyzed minimal bromate oscillator 219 (1994) 81
Sekine, R., see J. Onoe 217 (1994) 61
Sekine, S. and C. Hirose, Perturbation on intensity profiles of the CO 4pσ K $^1\Sigma^+$–3sσ B $^1\Sigma^+$(0–0) and 4pπ L $^1\Pi$–3sσ B $^1\Sigma^+$(0–0) bands 212 (1993) 129
Sekiya, H., T. Nakajima, H. Ujita, T. Tsuji, S. Ito and Y. Nishimura, Proton tunneling in tropolone–Rg (Rg=Ar, Kr, Xe) van der Waals complexes 215 (1993) 499
Sekiya, H., M. Habu, H. Ujita, T. Tsuji, A. Mori, H. Takeshita, Y. Nishimura, H. Petek and K. Yoshihara, Dual fluorescence and excited-state intramolecular proton transfer in jet-cooled 3,4-benzotropolone 215 (1993) 641
Sekkat, Z., M. Büchel, H. Orendi, H. Menzel and W. Knoll, Photoinduced alignment of azobenzene moieties in the side chains of polyglutamate films 220 (1994) 497
Selivanov, B.A., see V.A. Maltsev 212 (1993) 480
Selzle, H.L., see G.I. Nemeth 215 (1993) 151

Seminario, J.M., see P. Politzer 216 (1993) 348
Senekowitsch, J., see L.J. Brenner 215 (1993) 63
Sepp, W.-D., see T. Baştuğ 211 (1993) 119
Seraphin, S., D. Zhou, J. Jiao, M.A. Minke, S. Wang, T. Yadav and J.C. Withers, Catalytic role of nickel, palladium, and platinum in the formation of carbon nanoclusters 217 (1994) 191
Sergeev, A., see S. Hess 216 (1993) 247
Serrano-Andrés, L., M. Merchán, M. Fülscher and B.O. Roos, A theoretical study of the electronic spectrum of thiophene 211 (1993) 125
Seshadri, R., see D.V.S. Muthu 217 (1994) 146
Seshadri, R., see S.K. Ramasesha 220 (1994) 203
Seyfang, G., see H. Gross 213 (1993) 122
Seyfang, G., see Y. He 215 (1993) 228
Sha, G., see W. Sun 218 (1994) 515
Shafer, N.E., A.J. Orr-Ewing, W.R. Simpson, H. Xu and R.N. Zare, State-to-state differential cross sections from photoinitiated bulb reactions 212 (1993) 155
Shafizadeh, N., see S. Douin 216 (1993) 215
Shalabi, A.S. and A.M. El Misiery, Routes for LiF unit cell growth 215 (1993) 275
Shamrakov, D. and R. Reisfeld, Superradiant film laser operation in red perylimide dye doped silica–polymethylmethacrylate composite 213 (1993) 47
Shamshev, D.P., see N.N. Kudriavtsev 214 (1993) 513
Shapiro, M., Theory of the continuum excitation-emission spectrum of CH_3I 212 (1993) 444
Shashikala, M.N., see D.V.S. Muthu 217 (1994) 146
Shaw, A.M., see A. Carrington 212 (1993) 473
Shelton, D.P., see E.A. Donley 215 (1993) 156
Shen, Z.-X., see C.-H. Park 213 (1993) 196
Shestakov, O. and E.H. Fink, The a $^3\Sigma^+(a_1 1)$–X $^1\Sigma^+(X0^+)$ transition of BiN 211 (1993) 473
Shestakov, O., see R. Breidohr 218 (1994) 13
Sheu, W.-S. and P.J. Rossky, Dynamics of electron photodetachment from an aqueous halide ion 213 (1993) 233
Shi, F.G., Nonequilibrium inhomogeneous processes. An alternative mesoscopic description 212 (1993) 421
Shi, Z., J.V. Ford and A.W. Castleman Jr., Cluster reactions of sulfur trioxide and ammonia 220 (1994) 274
Shichida, Y., see H. Kandori 211 (1993) 385
Shima, T., see K. Ohta 217 (1994) 7
Shin, E., O.-K. Song, D. Kim, Y.D. Suh, S.I. Yang and S.K. Kim, Temperature-dependent Raman study on C_{70} film. Observation of a rotational ordering transition 218 (1994) 107
Shin, H.K., Importance of complex-mode collisions in the vibrational relaxation of strongly attracting molecules. The H_2O–HCl($v=1$) system 216 (1993) 27
Shinohara, H., see X.-D. Wang 216 (1993) 409
Shirley, D.A., see B.L. Petersen 213 (1993) 412; 220 (1994) 46
Shirley, D.A., see G. Remmers 214 (1993) 241
Shiromaru, H., see K. Kikuchi 216 (1993) 67
Shirsat, R.N., see S.R. Gadre 218 (1994) 593
Shkrob, I.A., see S.N. Batchelor 214 (1993) 507
Shkrob, I.A., see K.A. McLauchlan 217 (1994) 157
Shkrob, I.A., Spin-echo RYDMR. A theoretical examination 220 (1994) 347
Shore, J., see R.G. Larsen 214 (1993) 220
Shumway, J. and S. Satpathy, Polarization-dependent optical properties of C_{70} 211 (1993) 595

Sicilia, E., see N. Russo 213 (1993) 245
Siciliano, A., see V. Magnasco 213 (1993) 17
Sickafoose, S.M., see S.G. Kukolich 215 (1993) 168
Sidebottom, H.W., see C. Kelly 218 (1994) 29
Sidis, V., see B. Ramiro Diaz 212 (1993) 218
Siegbahn, P.E.M., see V.R. Jensen 212 (1993) 353
Siegbahn, P.E.M. and M. Svensson, Geometry optimization for second-row transition metal complexes 216 (1993) 147
Signorini, G.F., see C. Taiti 212 (1993) 283
Silbey, R., see A. Suárez 218 (1994) 445
Silbey, R.J., see G.M. Schmid 219 (1994) 331
Simard, B., see A.M. James 216 (1993) 512
Simon, J., see G. Guillaud 219 (1994) 123
Simon, J.D., see P. Cong 212 (1993) 367
Simons, J.P., see M. Baba 220 (1994) 411
Simpson, C.J.S.M., see G.J. Wilson 214 (1993) 297
Simpson, W.R., see N.E. Shafer 212 (1993) 155
Simpson, W.R., A.J. Orr-Ewing and R.N. Zare, State-to-state differential cross sections for the reaction $Cl(^2P_{3/2}) + CH_4(\nu_3 = 1, J = 1) \rightarrow HCl(v' = 1, J') + CH_3$ 212 (1993) 163
Sims, I.R., J.-L. Queffelec, D. Travers, B.R. Rowe, L.B. Herbert, J. Karthäuser and I.W.M. Smith, Rate constants for the reactions of CN with hydrocarbons at low and ultra-low temperatures 211 (1993) 461
Singh, A.K., see S.K. Ramasesha 220 (1994) 203
Singh, R.K., B.P. Asthana and H.D. Bist, Study of the dynamics of phase transition in NH_4SCN by a precise Raman linewidth and frequency shift measurement (Chem. Phys. Letters 209 (1993) 390). Erratum 213 (1993) 210
Singleton, S.M. and R.D. Coombe, Rate and mechanism of the $NH(a\ ^1\Delta) + Cl_2$ reaction 215 (1993) 237
Sinha, A., see D.E. Govoni 216 (1993) 525
Sinha, H.K. and R.P. Steer, S_2–S_0 fluorescence excitation spectroscopy of van der Waals complexes of xanthione and benzopyranthione with N_2 and CO 211 (1993) 397
Siska, P.E., see M.F. Falcetta 213 (1993) 531
Sixl, H., see A. Angerhofer 217 (1994) 403
Sizaret, P.-Y., see B. Keita 215 (1993) 125
Skiebe, A., A. Hirsch, H. Klos and B. Gotschy, $[DBU]C_{60}$. Spin pairing in a fullerene salt 220 (1994) 138
Skourtis, S.S. and J.N. Onuchic, Effective two-state systems in bridge-mediated electron transfer. A Green function analysis (Chem. Phys. Letters 209 (1993) 171). Erratum 211 (1993) 282
Skurat, V.E., see A.P. Nikiforov 212 (1993) 43
Smeyers, Y.G., see V. Botella 219 (1994) 497
Smirnov, S.N. and C.L. Braun, Light polarization effects in the transient dc conductivity response to excitation of dipolar solutes 217 (1994) 167
Smirnov, V.V., see M. Ehbrecht 214 (1993) 34
Smit, T.S. and K.H. Johnson, Hydrodesulphurization of thiophene by transition metal sulphides. A molecular orbital topology study 212 (1993) 525
Smith, D. and P. Španel, Dissociative recombination of H_3^+. Experiment and theory reconciled 211 (1993) 454
Smith, D., P. Španel and T.D. Märk, Electron attachment to C_{60} at low energies 213 (1993) 202

Smith, D.M., R.P. Tuckett, K.R. Yoxall, K. Codling and P.A. Hatherly, Fragmentation of the $\tilde{C}\ ^2T_2$ and $\tilde{D}\ ^2A_1$ states of CCl_4^+ and $SiCl_4^+$ studied by threshold photoelectron–photoion coincidence spectroscopy 216 (1993) 493
Smith, I.W.M., see I.R. Sims 211 (1993) 461
Smith, M.E., C. Jaeger, R. Schoenhofer and S. Steuernagel, Structural characterisation of the aluminium sites in kyanite by ^{27}Al magic angle spinning centreband, satellite transition and double rotation NMR 219 (1994) 75
Smith, P.E. and W.F. Van Gunsteren, The viscosity of SPC and SPC/E water at 277 and 300 K 215 (1993) 315
Smith, P.G., see T. Troxler 211 (1993) 371
Smith, W.W., see C. Tapalian 211 (1993) 425
Smith Jr., V.H., see M. Hô 219 (1994) 15
Smith Jr., V.H., see J. Wang 220 (1994) 331
Snyder, G. and D. Sapse, Ab initio studies of complexes of ozone with some positive ions 218 (1994) 372
Sobolewski, A.L. and W. Domcke, Evidence for the need of a non-Born–Oppenheimer description of excited-state hydrogen transfer 211 (1993) 82
Sobolewski, A.L., The mechanism of excited-state hydrogen transfer in 2-hydroxypyridine 211 (1993) 293
Sodupe, M. and C.W. Bauschlicher Jr., A theoretical study of the spectroscopy of SrH_2O^+ and $SrNH_3^+$ 212 (1993) 624
Sodupe, M., see C.W. Bauschlicher Jr. 214 (1993) 489
Solé, A., see A. Aguilar 220 (1994) 267
Solgadi, D., see S. Martrenchard-Barra 215 (1993) 291
Sominska, E., V. Kelner and A. Gedanken, Is the Schumann–Runge continuum of oxygen structureless? 213 (1993) 117
Song, O.-K., see E. Shin 218 (1994) 107
Song, X., Y. Bao, R.S. Urdahl, J.N. Gosine and W.M. Jackson, Laser-induced fluorescence studies of C_3 formation and isomerization in the 193 nm photolysis of allene and propyne 217 (1994) 216
Song, Z., R. Lu, N. Lou and R. Zhai, The effect of exchange process on the kinetics of desorption and adsorption of CO on Rh(111) surface 217 (1994) 142
Song, Z., see M. Ohashi 220 (1994) 7
Sood, A.K., see D.V.S. Muthu 217 (1994) 146
Sood, A.K., see S.K. Ramasesha 220 (1994) 203
Sosa, C., C. Lee, G. Fitzgerald and R.A. Eades, Chemical applications of density functional theory: F_3^- anion dissociation ($F_3^- \rightarrow F_2 + F^-$) 211 (1993) 265
Soscun, H., see P.J. O'Malley 217 (1994) 293
Soscun Machado, H.J., see A. Hinchliffe 214 (1993) 64
Sousa, C., F. Illas, C. Bo and J.M. Poblet, Topological analysis of charge density in ionic solids 215 (1993) 97
Španel, P., see D. Smith 211 (1993) 454; 213 (1993) 202
Spano, F.C., Mean-field nonlinear optical susceptibility of charge-transfer crystals 211 (1993) 491
Spano, F.C., Theory of strong-field pump–probe spectroscopy in J-aggregates 220 (1994) 365
Spielfiedel, A., N. Feautrier, G. Chambaud, P. Rosmus and H.-J. Werner, The first dipole-allowed electronic transition $1\ ^1\Sigma_u^+ – X\ ^1\Sigma_g^+$ of CO_2 216 (1993) 162
Spiess, H.W., see H. Geen 213 (1993) 145
Spiess, H.W., see M. Hubrich 218 (1994) 81
Spitchina, N.G., see M.V. Motyakin 216 (1993) 63
Squires, R.R., see L.S. Sunderlin 212 (1993) 307

Squitieri, E., see J.L. Paz 217 (1994) 333
Sremaniak, L.S., L. Perera and M.L. Berkowitz, Enthalpies of formation and stabilization energies of $Br^-(H_2O)_n$ ($n=1, 2, ..., 15$) clusters. Comparisons between molecular dynamics computer simulations and experiment 218 (1994) 377
Stahl, T., see H. Lanig 220 (1994) 423
Stair, P.C., see S.J. Garrett 219 (1994) 409
Stammler, W., see S. Schneider 219 (1994) 433
Stankevich, I.V., see E.G. Gal'pern 214 (1993) 345
Stassen, H. and Z.E. Gburski, Instantaneous normal mode analysis of binary liquid Ar–Kr mixtures 217 (1994) 325
Steele, W.A., see S.I. Temkin 215 (1993) 285
Steer, R.P., see H.K. Sinha 211 (1993) 397
Stehlik, D., see A. Van der Est 212 (1993) 561
Stehlik, D., see I.Y. Chan 219 (1994) 187
Stelmakh, O., see M. Ehbrecht 214 (1993) 34
Stensgaard, I., see M. Foss 215 (1993) 535
Stenson, C., see A.B. Finnila 219 (1994) 343
Stenzel, W., see M. Ondřejček 215 (1993) 528
Stepanov, A.G., see I.V. Bezel 218 (1994) 475
Stepanov, N.F., see A.A. Buchachenko 220 (1994) 93
Stephens, R.L., see P. Schwerdtfeger 218 (1994) 362
Sterk, H., see R. Konrat 212 (1993) 78
Steuernagel, S., see M.E. Smith 219 (1994) 75
Stich, I., see D.M. Bird 212 (1993) 518
Štich, I., M.C. Payne, A. De Vita, M.J. Gillan and L.J. Clarke, Chemically driven molecular decomposition at semiconductor surfaces 212 (1993) 617
Stickel, R.E., Z. Zhao and P.H. Wine, Branching ratios for hydrogen transfer in the reactions of OD radicals with CH_3SCH_3 and $CH_3SC_2H_5$ 212 (1993) 312
Stief, L.J., see P.S. Monks 211 (1993) 416
Stockman, P.A. and G.A. Blake, HF...Cl_2. Bending dynamics of an antihydrogen-bonded van der Waals dimer 212 (1993) 298
Stoeckel, F., see A. Charvát 214 (1993) 495
Stohner, J., see D. Luckhaus 212 (1993) 434
Stolarczyk, L.Z., Complete active space coupled-cluster method. Extension of single-reference coupled-cluster method using the CASSCF wavefunction 217 (1994) 1
Stoll, H., see E. Czuchaj 212 (1993) 534; 218 (1994) 454
Stoll, H., see J. Gräfenstein 215 (1993) 611
Stoll, H., see D. Andrae 220 (1994) 341
Stolte, S., see G. van den Hoek 215 (1993) 461
Stolte, S., see A.E. Wiskerke 216 (1993) 93
Stolte, S., see C.A. Taatjes 216 (1993) 100
Stone, A.J., Computation of charge-transfer energies by perturbation theory 211 (1993) 101
Storer, J.W., see C.J. Cramer 218 (1994) 387
Stranges, D., see N. Balucani 211 (1993) 469
Stringat, R., G. Fabre, M. El Ajli and R. Bacis, Time-selected spectra in Fourier transform spectrometry of pulsed sources 220 (1994) 429
Strömholm, C., see P. Erman 215 (1993) 173

Strout, D.L., see K. Raghavachari 214 (1993) 357
Strout, D.L., R.L. Murry, C. Xu, W.C. Eckhoff, G.K. Odom and G.E. Scuseria, A theoretical study of buckminsterfullerene reaction products: $C_{60}+C_{60}$ 214 (1993) 576
Struganova, I.A., see V.F. Kamalov 213 (1993) 559; 220 (1994) 257
Studer, S.L., see P.-T. Chou 216 (1993) 300
Stuhl, F., see J. Hohmann 217 (1994) 577
Stuhlmann, C., I. Villegas and M.J. Weaver, Scanning tunneling microscopy and infrared spectroscopy as combined in situ probes of electrochemical adlayer structure. Cyanide on Pt(111) 219 (1994) 319
Stwalley, W.C., see L.N. Ding 212 (1993) 499
Su, Y., see J.S. Francisco 215 (1993) 58, 417
Su, Z.-B., see S. Qin 213 (1993) 373
Suárez, A. and R. Silbey, Low-temperature dynamics in glasses and the stochastic sudden-jump model 218 (1994) 445
Subbaswamy, K.R., see M. Menon 219 (1994) 219
Subramanian, G., E.D. Jemmis and B.V. Prasad, Ab initio MO studies on the isomers of Si_2BH_3 217 (1994) 296
Suga, H., see Y. Miyazaki 213 (1993) 303
Sugioka, T., see A. Nakajima 214 (1993) 22
Suh, Y.D., see E. Shin 218 (1994) 107
Suhm, M.A., Multidimensional vibrational quantum Monte Carlo technique using robust interpolation from static or growing sets of discrete potential energy points 214 (1993) 373
Sukhov, A.M., see N.N. Kudriavtsev 214 (1993) 513
Sullivan, D.E., see A.R. Denton 219 (1994) 310
Sülzle, D., see N. Goldberg 213 (1993) 593
Sumithra, G., see V. Nagalakshmi 217 (1994) 279
Sumiyama, K., see Y. Saito 212 (1993) 379
Sumiyoshi, Y., K. Tanaka and T. Tanaka, Infrared diode laser spectroscopy of the $SiCl^+$ ion 214 (1993) 17
Sun, H., see J.K. Park 211 (1993) 618
Sun, W., G. Sha, B. Jiang, E.J. Hintsa and C. Zhang, *M*- and e/f-symmetry-resolved cross sections for CO(A $^1\Pi$)–He/Ar collision-induced energy transfer from $J=2$ to $J=1$ 218 (1994) 515
Sun, W., see G. Ding 220 (1994) 1
Sun, Z.-J., A.L. Schwaner and J.M. White, Photoinduced charge transfer at surfaces: CF_3I adsorbed on Ag(111) 219 (1994) 118
Sunderlin, L.S. and R.R. Squires, Determination of the H_2O–NO_2^+ and $CH_3O(H)$–NO_2^+ bond strengths and the proton affinities of nitric acid and methyl nitrate 212 (1993) 307
Sundholm, D. and J. Olsen, Core–valence correlation effects on the ground state electron affinity of calcium 217 (1994) 451
Sundqvist, B.U.R., see P.A. Brühwiler 214 (1993) 45
Sundström, G., M. Carlson, M. Larsson and L. Broström, High-resolution spectroscopy of the A $^1\Pi_u$–X $^1\Sigma_g^+$ (6, 1) band in N_2^{2+} 218 (1994) 17
Sundström, V., see U. Åberg 215 (1993) 388
Sundström, V., see S. Hess 216 (1993) 247
Suppan, P., see E. Vauthey 215 (1993) 264
Supronowicz, J., M.J. Hinek, J.B. Atkinson and L. Krause, Mixing of the Cd 5^3P fine-structure states by Hg collisions 213 (1993) 282

Supronowicz, J., E. Hegazi, J.B. Atkinson and L. Krause, Laser spectroscopy of some high-lying HgZn spin–orbit states 218 (1994) 240
Supronowicz, J., see W. Kedzierski 218 (1994) 314
Suter, D., see T. Blasberg 215 (1993) 668
Suter, U.W., see M. Tomaselli 214 (1993) 1
Suvernev, A.A. and T. Dreier, Evaluation of CARS spectra. Spectra of symmetric molecules in the Keilson–Storer model 216 (1993) 1
Suvernev, A.A. and T. Dreier, Evaluation of CARS spectra. Doppler broadening in spectra of linear molecules 216 (1993) 5
Suwaiyan, A., see K.A. Al-Hassan 212 (1993) 581
Suwaiyan, A., see U.K.A. Klein 217 (1994) 80, 86
Suzuki, K., see Y. Saito 212 (1993) 379
Suzuki, S., see K. Kikuchi 216 (1993) 67
Svensson, M., see P.E.M. Siegbahn 216 (1993) 147
Svirko, Yu.P., see A.R. Bungay 217 (1994) 249
Svishchev, I.M. and P.G. Kusalik, Roto–translational motion in liquid water and its structural implication 215 (1993) 596
Swiech, W., see B. Rausenberger 215 (1993) 109
Sworakowski, J., K. Palewska and M. Bertault, A calorimetric study of phase transitions in C_{70} fullerene 220 (1994) 197
Syage, J.A., Predissociation lifetimes of the $\tilde{B}$ and $\tilde{C}$ Rydberg states of CH_3I 212 (1993) 124
Szalay, P.G. and R.J. Bartlett, Multi-reference averaged quadratic coupled-cluster method: a size-extensive modification of multi-reference CI 214 (1993) 481
Szente, J.J., see M.M. Maricq 213 (1993) 449; 220 (1994) 243
Szmytkowski, C., see A.M. Krzysztofowicz 219 (1994) 86
Szwarc, H., see B. Keita 215 (1993) 125

Taatjes, C.A., see G. van den Hoek 215 (1993) 461
Taatjes, C.A., see A.E. Wiskerke 216 (1993) 93
Taatjes, C.A., J.W.G. Mastenbroek and S. Stolte, Vibrational and rotational effects on fragmentation of CF_3I via (2+1) resonance-enhanced multiphoton ionization 216 (1993) 100
Tachikawa, E., see Y. Fujitani 214 (1993) 301
Tachikawa, H., Reaction mechanism of the radical isomerization from CH_3O to CH_2OH in frozen methanol. An ab initio MO and RRKM study 212 (1993) 27
Tachiya, M., see A.V. Barzykin 216 (1993) 575
Tachiya, M., see S. Murata 219 (1994) 200
Tadjeddine, A., see A. Peremans 220 (1994) 481
Taguwa, T., see A. Nakajima 214 (1993) 22
Tahara, T. and H. Hamaguchi, Transient Raman spectra and structure of the "twisted" excited singlet state of tetraphenylethylene 217 (1994) 369
Tahara, T., see T. Tsukuda 218 (1994) 1
Taiji, M., see K. Minoshima 218 (1994) 67
Taiti, C., P. Foggi, G.F. Signorini and V. Schettino, Vibrational relaxation of a MnO_4^- impurity mode in $KClO_4$ crystal 212 (1993) 283
Takada, T., see M. Tomonari 215 (1993) 45
Takagi, N., see J. Yoshinobu 211 (1993) 48
Takagi, N., J. Yoshinobu and M. Kawai, Direct observation of isothermal adsorption and desorption processes of CO on the Ni(100) surface 215 (1993) 120
Takahashi, A., H.X. Wang and S. Mukamel, Collective charge density fluctuations and nonlinear optical response of C_{60} 216 (1993) 394
Takahashi, H., see J. Watanabe 213 (1993) 351
Takahashi, T., see A. Ito 211 (1993) 333
Takahashi, T., see T. Nakayama 215 (1993) 622
Takaichi, S., see M. Mimuro 213 (1993) 576
Takano, K., see H. Umemoto 214 (1993) 271
Takaoka, T., Y. Yasui, M. Sawada, T. Aruga and M. Nishijima, Coadsorption of CO and C_2H_4 on Pd(110). Formation of a (3×2) mixed structure 215 (1993) 523
Takasu, R., Y. Fujiwara and M. Itoh, No excited state proton transfer takes place in jet-cooled methanol clusters of 3-hydroxyflavone 217 (1994) 478
Takayanagi, M., see T. Gejo 218 (1994) 343
Takeda, J., T. Tayu, S. Kurita, Y. Yokoyama, Y. Kurita, T. Kuga and M. Matsuoka, Radiative and non-radiative decay processes of the excited state of the colored form of photochromic furylfulgide 220 (1994) 443
Takeda, Y., see F. Mafuné 218 (1994) 234
Takeshita, H., see H. Sekiya 215 (1993) 641
Takeuchi, K., see J. Onoe 217 (1994) 61
Talapatra, G.B., see A.K. Dutta 212 (1993) 637
Taliani, C., see F. Negri 211 (1993) 353
Taliani, C., see O. Dippel 216 (1993) 418
Taliani, C., see F. Kajzar 217 (1994) 418
Tamai, N., C.F. Porter and H. Masuhara, Femtosecond transient absorption spectroscopy of a single perylene microcrystal under a microscope 211 (1993) 364
Tamai, N., see S. Hamai 213 (1993) 407
Tamassia, F., see C. Degli Esposti 214 (1993) 531

Tamura, T., see Y. Fujiwara 213 (1993) 89
Tanabe, S., T. Ebata, M. Fujii and N. Mikami, OH stretching vibrations of phenol–$(H_2O)_n$ ($n=1$–3) complexes observed by IR–UV double-resonance spectroscopy 215 (1993) 347
Tanaka, A., see K. Yamasaki 215 (1993) 483
Tanaka, H., The thermodynamic stability of clathrate hydrate. Encaging non-spherical propane molecules 220 (1994) 371
Tanaka, K., see Y. Matsuzaki 211 (1993) 300
Tanaka, K., see K. Yoshizawa 213 (1993) 498
Tanaka, K., see Y. Sumiyoshi 214 (1993) 17
Tanaka, K., see H. Ikeura 217 (1994) 131
Tanaka, K., see K. Okahara 219 (1994) 462
Tanaka, T., see Y. Sumiyoshi 214 (1993) 17
Tanaka, Y., see A. Osuka 215 (1993) 179
Tang, A.-C. and Q.-S. Li, Eigenvalues and eigenfunctions of Hückel Hamiltonian for carbon species with D_p or D_{ph} symmetry 212 (1993) 391
Tang, J., Superexchange electron-transfer reactions in a three-component system. The spin-boson model for photosynthesis 217 (1994) 55
Tang, J., M.C. Thurnauer and J.R. Norris, Electron spin echo envelope modulation due to exchange and dipolar interactions in a spin-correlated radical pair 219 (1994) 283
Tang, K., see R.B. Jones 212 (1993) 451
Tani, T., see V.F. Kamalov 220 (1994) 257
Tanigaki, K., I. Hirosawa, J. Mizuki and T.W. Ebbesen, Lattice parameters of alkali-metal-doped C_{60} fullerides 213 (1993) 395
Tanimoto, Y., see Y. Fujiwara 213 (1993) 89
Tapalian, C. and W.W. Smith, Triatomic associative ionization: Na_3^+ formation 211 (1993) 425
Tars, M., see A. Freiberg 214 (1993) 10
Tasumi, M., see R. Inaba 211 (1993) 183
Tayu, T., see J. Takeda 220 (1994) 443
Tchénio, P., A.B. Myers and W.E. Moerner, Vibrational analysis of the dispersed fluorescence from single molecules of terrylene in polyethylene 213 (1993) 325
Tchougreeff, A.L., The origin of cooperativity in high-spin–low-spin transitions in molecular crystals 214 (1993) 627
Teixeira-Dias, J.J.C., see R.D. Gordon 211 (1993) 392
Tekely, P., see D. Canet 212 (1993) 483
Temkin, S.I. and W.A. Steele, MD simulation of rotational relaxation in liquid nitrogen. Comparison with NMR and Raman data 215 (1993) 285
Ten-no, S., An efficient algorithm for electron repulsion integrals over contracted Gaussian-type functions 211 (1993) 259
Ten-no, S., F. Hirata and S. Kato, A hybrid approach for the solvent effect on the electronic structure of a solute based on the RISM and Hartree–Fock equations 214 (1993) 391
Terazima, M. and N. Hirota, Time-resolved two-step excitation thermal grating method. Measurement of the quantum yield of energy transfer from a higher excited triplet state 214 (1993) 541
Terazima, M., Measurement of translational diffusion of a photochemically stable molecule by the transient grating method. Hematoporphyrin in acetone 218 (1994) 574
Terletski, C., see C.P.M. Giesbergen 213 (1993) 597
Terlouw, J.K., see G.A. McGibbon 218 (1994) 499
Ter Meer, H.U., see A. Angerhofer 217 (1994) 403

Ter Meulen, J.J., see G. Hilpert 219 (1994) 384
Terminello, L.J., see B.L. Petersen 213 (1993) 412; 220 (1994) 46
Thantu, N. and P.M. Weber, Dependence of two-photon ionization photoelectron spectra on laser coherence bandwidth 214 (1993) 276
Thelen, M.-A., P. Felder and J.R. Huber, The photofragmentation of methyl hydroperoxide CH_3OOH at 193 and 248 nm in a cold molecular beam 213 (1993) 275
Thewalt, M.L.W., see P.J. Horoyski 217 (1994) 409
Thiel, P.A., see M.R. Columbia 220 (1994) 167
Thiel, W., see C. Heinemann 217 (1994) 11
Thiem, T.L., R.H. Salter and J.A. Gardner, The velocity/kinetic energy distributions of Sc and ScO and optical spectra from the laser vaporization of Sc_2O_3 218 (1994) 309
Thoma, A., see N. Caspary 212 (1993) 329
Thoma, A., see G. Schallmoser 219 (1994) 101
Thomas, J.M. and D.H. Katayama, Branching fractions of the product NO($A\ ^2\Sigma^+$, $v=0$, 1) and NO($B\ ^2\Pi_r$, $v=0$) emissions observed as a function of v' in the energy transfer reaction $N_2(A\ ^3\Sigma_u^+, v') + NO(X\ ^2\Pi_r, v''=0)$ 214 (1993) 250
Thompson, D.L., see K.L. Bintz 215 (1993) 455
Thompson, D.L., see C.C. Chambers 218 (1994) 166
Thomsen, C., see L. Akselrod 212 (1993) 384; 215 (1993) 131
Thomsen, E.L., O.J. Nielsen and H. Egsgaard, The reaction of nitromethane with hydrogen and deuterium atoms in the gas phase. A mechanistic study 215 (1993) 257
Thorn, J.C., see A.C. Legon 215 (1993) 554
Thurnauer, M.C., see J. Tang 219 (1994) 283
Timonen, R.S., see A.A. Iogansen 212 (1993) 604
Timpmann, K., see A. Freiberg 214 (1993) 10
Tinker, F.A., see L. Nemes 218 (1994) 295
Tinti, D.S., see S.M. Neugebauer 211 (1993) 555
Tipikin, D.S., Ya.S. Lebedev, O.G. Poluektov and J. Schmidt, ESE-detected EPR of triplet radical pairs produced by mechano-chemical treatment of 2,6-di-*t*-butylquinone diazide mixed with 3,5-di-*t*-butylpyrocathechon 215 (1993) 199
Tipikin, D.S., see S.D. Chemerisov 218 (1994) 353
Titman, J.J., see H. Geen 213 (1993) 145
Todorović, D., see I. Gutman 216 (1993) 447
Tokmakoff, A., see D.R. Haynes 214 (1993) 50
Tokue, I., see K. Yamasaki 215 (1993) 483
Tokumaru, K., see T. Arai 212 (1993) 597
Toleno, B.J., see S.F. Cartier 220 (1994) 23
Tomás, F., see M.C. Piqueras 213 (1993) 509
Tomaselli, M., B.H. Meier, P. Robyr, U.W. Suter and R.R. Ernst, Direct measurement of xenon exchange between gas and liquid phase by 2D NMR 214 (1993) 1
Tomer, J.L., M.C. Wall, B.P. Reid and J.I. Cline, Photofragmentation dynamics of 2-chloro-2-nitrosopropane. Scalar correlations of velocity and angular momentum 216 (1993) 286
Tominaga, K., see R. Inaba 211 (1993) 183
Tomioka, H., see H. Kandori 211 (1993) 385
Tomonari, M., N. Ookubo and T. Takada, Missing-orbital analysis of molecular hyperpolarizability β calculated by a simplified sum-over-states method. Enhancement of the off-diagonal component β_{zxx} 215 (1993) 45

Topp, M.R., see T. Troxler 211 (1993) 371
Tordo, P., see G.G. Lazarev 212 (1993) 319
Torre, R., I. Sánta and R. Righini, Pre-transitional effects in the liquid–plastic phase transition of *p*-terphenyl 212 (1993) 90
Törring, T., see J. Hoeft 215 (1993) 367
Toscano, M., see N. Russo 213 (1993) 245
Tossell, J.A., see D.C. Winkler 219 (1994) 57
Tossell, J.A., The relationship between the inner-shell electron energy-loss spectra and the ^{29}Si NMR spectra of the chlorosilanes, SiH_xCl_{4-x}. An interpretation of the trend in NMR shieldings 219 (1994) 65
Totrov, M.M., see M.M. Triebel 214 (1993) 315, 321
Trache, M., see F.M. Bénière 215 (1993) 301
Tramer, A., see M. Chergui 216 (1993) 34
Tran-Thi, T.-H., T. Fournier, A. De Cian, D. Chabach, R. Weiss, D. Houde, C. Pépin and L. Dao, Picosecond relaxation of charge transfer states in an asymmetric cerium double-decker sandwich compound 213 (1993) 139
Travers, D., see I.R. Sims 211 (1993) 461
Treacy, J., see C. Kelly 218 (1994) 29
Trebino, R., see J.A. Gray 216 (1993) 519
Tributsch, H., see D. Haneman 216 (1993) 81
Triebel, M.M., M.M. Totrov, G.E. Zorinyants and E.L. Frankevich, The use of the magnetic field effect for studying a chemiluminescent chemical reaction in aqueous solution. Reaction rate constants and lifetimes of intermediate molecules 214 (1993) 315
Triebel, M.M., A.K. Morozov, M.M. Totrov, G.E. Zorinyants and E.L. Frankevich, Phase-on-frequency characteristics of the magnetic field effect for studying the mechanism of the branching chemiluminescent reaction of luminol 214 (1993) 321
Trifunac, A.D., see K.R. Cromack 218 (1994) 485
Troe, J., see J. Schroeder 218 (1994) 43
Trommsdorff, H.P., see S. Astilean 219 (1994) 95
Tronc, M., see R. Azria 220 (1994) 417
Tronchet, J.M.J., see I. Komaromi 215 (1993) 444
Troxler, T., P.G. Smith and M.R. Topp, Structural measurements of hydrogen-bonded van der Waals dimers and trimers by rotational coherence spectroscopy. 2,5-diphenyloxadiazole (PPD) with water 211 (1993) 371
Trubnikov, D.N., see A.V. Larin 213 (1993) 619
Truhlar, D.G., see S.L. Mielke 213 (1993) 10; 216 (1993) 441; 217 (1994) 173
Truong, T.N., see T.A. Holme 215 (1993) 53
Truttmann, L., see T. Bally 212 (1993) 141
Tsai, C.J. and K.D. Jordan, Theoretical study of the $(H_2O)_6$ cluster 213 (1993) 181
Tse, J.S., B.M. Powell, V.F. Sears and Y.P. Handa, The lattice dynamics of clathrate hydrates. An incoherent inelastic neutron scattering study 215 (1993) 383
Tsokos, E., see K. Pierloot 214 (1993) 583
Tsuchioka, T., see Y. Kohno 214 (1993) 603
Tsuji, T., see H. Sekiya 215 (1993) 499, 641
Tsukerblat, B.S., see J.J. Borrás-Almenar 217 (1994) 525
Tsukiyama, K., see J. Ishii 220 (1994) 29
Tsukuda, T., M. Nagaminé, T. Tahara, T. Nagata and T. Kondow, Competitive electron capture in mixed clusters, $X(HCN)_m$ ($X = C_2H_5OH$, CO_2, O_2, and SF_6) 218 (1994) 1

Tsunashima, S., see H. Umemoto 214 (1993) 271
Tsunashima, S., see A. Masaki 218 (1994) 523
Tuckett, R.P., see D.M. Smith 216 (1993) 493
Turnidge, M.L., see G.J. Wilson 214 (1993) 297

Uehara, H., K. Horiai, A. Kerim, Y. Ozaki and T. Konno, Infrared emission spectrum of NaBr 213 (1993) 101
Uehara, H., K. Horiai, Y. Ozaki and T. Konno, Infrared emission spectrum of AlBr 214 (1993) 527
Uehara, H., K. Horiai, Y. Ozaki and T. Konno, Infrared diode laser spectroscopy of high-temperature molecules using spectrum processing by Fourier transformation 215 (1993) 505
Uehara, K., see J. Ishii 220 (1994) 29
Ugarte, D., see W.S. Bacsa 211 (1993) 346
Ugliengo, P., see A.M. Ferrari 212 (1993) 644
Ujita, H., see H. Sekiya 215 (1993) 499, 641
Ukitsu, M., see K. Yoshikawa 211 (1993) 211
Ulrich, K., see J. Walz 213 (1993) 321
Umanskii, I.M., see S.I. Vetchinkin 215 (1993) 11
Umapathy, S., see C. Engert 218 (1994) 87
Umemoto, H., T. Sato, K. Takano, S. Tsunashima, K. Kuwahara, K. Sato, H. Ikeda, F. Misaizu and K. Fuke, Nascent rotational state distributions of ZnH($X\ ^2\Sigma^+$) produced in the reactions of Zn($4\ ^1P_1$) with simple alkane hydrocarbons 214 (1993) 271
Uosaki, K., see S. Nakabayashi 217 (1994) 163
Urdahl, R.S., see M. Gong 217 (1994) 210
Urdahl, R.S., see X. Song 217 (1994) 216

Vacek, J., K. Konvička and P. Hobza, A molecular dynamics study of the benzene...Ar_2 complex. Application of the nonempirical ab initio and empirical Lennard-Jones 6–12 potentials 220 (1994) 85
Vachev, V.D., J.H. Frederick, B.A. Grishanin, V.N. Zadkov and N.I. Koroteev, Stilbene isomerization dynamics on multidimensional potential energy surface. Molecular dynamics simulation 215 (1993) 306
Vahtras, O., J. Almlöf and M.W. Feyereisen, Integral approximations for LCAO-SCF calculations 213 (1993) 514
Vaida, V., see K.O. Lantz 215 (1993) 329
Valdry, L., see V.R. Morris 220 (1994) 448
Valent, I. and L. Adamčíková, The clock behavior of the BrO_3^-–SCN^- reaction 216 (1993) 479
Valentini, J.J., see D.V. Lanzisera 216 (1993) 122
Van den Hoek, G., M. Jonker, D.H. Parker, C.A. Taatjes and S. Stolte, Double-resonance measurements of vibrational levels populated by infrared multiphoton excitation of CF_3I in a molecular beam 215 (1993) 461
Van der Auweraer, M., see S. Depaemelaere 215 (1993) 649
Vanderbilt, D., see F. Liu 215 (1993) 401
Van der Est, A., R. Bittl, E.C. Abresch, W. Lubitz and D. Stehlik, Transient EPR spectroscopy of perdeuterated Zn-substituted reaction centres of *Rhodobacter sphaeroides* R-26 212 (1993) 561
Van der Laan, H., C. De Caro, Th. Schmidt, R.W. Visschers, R. van Grondelle, G.J.S. Fowler, C.N. Hunter and S. Völker, Excited-state dynamics of mutated antenna complexes of purple bacteria studied by hole-burning 212 (1993) 569
Van der Maarel, J.R.C., see T.W.N. Bieze 216 (1993) 56
Van der Sijs, D.A., E.E. van Faassen and Y.K. Levine, The interpretation of fluorescence anisotropy decays of probe molecules in membrane systems 216 (1993) 559
Van Dijk, S.I., P.G. Wiering, R. van Staveren, H.J. van Ramesdonk, A.M. Brouwer and J.W. Verhoeven, Two-step photoinduced charge separation and unexpectedly fast one-step charge recombination in a linked $donor_2$–$donor_1$–acceptor system 214 (1993) 502
Van Enckevort, W.J.P., see M.A. Verheijen 216 (1993) 72
Van Faassen, E.E., see D.A. van der Sijs 216 (1993) 559
Van Grondelle, R., see H. van der Laan 212 (1993) 569
Van Gunsteren, W.F., see P.E. Smith 215 (1993) 315
Vanquickenborne, L.G., see M.T. Nguyen 212 (1993) 543
Van Ramesdonk, H.J., see S.I. van Dijk 214 (1993) 502
Van Santen, R.A., see M.J.P. Brugmans 217 (1994) 117
Van Smaalen, S., see J.L. de Boer 219 (1994) 469
Van Staveren, R., see S.I. van Dijk 214 (1993) 502
Van Wüllen, C., An implementation of a Kohn–Sham density functional program using a Gaussian-type basis set. Application to the equilibrium geometry of C_{60} and C_{70} 219 (1994) 8
Van Zee, R.J., S. Li and W. Weltner Jr., Ground electronic states of ZrO^+, HfO^+, and Nb_2^+. ESR spectra of the matrix-isolated ions 217 (1994) 381
Vauthey, E., D. Pilloud, E. Haselbach, P. Suppan and P. Jacques, The reliability of free ion yield in photoinduced electron transfer reactions. The model system 9,10-dicyanoanthracene/biphenyl in acetonitrile 215 (1993) 264
Vauthey, E., Picosecond transient grating study of the reorientation dynamics of nile red in different classes of solvent 216 (1993) 530
Veeman, W.S., see M. Mansfeld 213 (1993) 153

Velasco, S., see J.M.M. Roco 216 (1993) 593
Ventura, O.N., K. Irving and Z. Latajka, The dimerization shift of the OH-stretching fundamentals of the water dimer 217 (1994) 436
Venuti, E., see A. Brillante 218 (1994) 568
Verdún, H.R., see U. Hömmerich 213 (1993) 163
Vergès, J., see R.F. Barrow 214 (1993) 293
Verheijen, M.A., see M. Matsushita 214 (1993) 349
Verheijen, M.A., W.J.P. van Enckevort and G. Meijer, Growth phenomena on C_{60} crystals 216 (1993) 72
Verheijen, M.A., see J.L. de Boer 219 (1994) 469
Verhoeven, J.W., see S.I. van Dijk 214 (1993) 502
Verhoeven, J.W., see S. Depaemelaere 215 (1993) 649
Veszprémi, T., see T. Pasinszki 215 (1993) 395
Vetchinkin, A.S., see S.I. Vetchinkin 215 (1993) 11
Vetchinkin, S.I., A.S. Vetchinkin, V.V. Eryomin and I.M. Umanskii, Gaussian wavepacket dynamics in an anharmonic system 215 (1993) 11
Viaene, L., see S. Depaemelaere 215 (1993) 649
Vialle, J.L., see M. Pellarin 217 (1994) 349
Viant, M.R., see A. Carrington 212 (1993) 473
Vigil, L.E., see M.C. Schneebeck 215 (1993) 251
Vijayakumar, M., S. Roszak and K. Balasubramanian, An efficient relativistic multireference configuration interaction method 215 (1993) 87
Vilesov, A.F., see Ch. Ottinger 211 (1993) 175
Vilesov, A.F., see A.A. Matveev 217 (1994) 582
Villegas, I., see C. Stuhlmann 219 (1994) 319
Vinogradov, An.V., see J. Janszky 213 (1993) 368
Visschers, R.W., see H. van der Laan 212 (1993) 569
Vlachy, V., see Yu.V. Kalyuzhnyi 215 (1993) 518
Voda, M., see U. Caldiño G. 213 (1993) 84
Vogel, E., see A. Berman 211 (1993) 549
Vögtle, F., see S. Grimme 213 (1993) 32
Vöhringer, P., see J. Schroeder 218 (1994) 43
Vojtík, J., A new theoretical approach to collision-induced autoionization in atom–diatom systems with repulsive interactions 214 (1993) 425
Völker, S., see H. van der Laan 212 (1993) 569
Volpi, G.G., see N. Balucani 211 (1993) 469
Volpp, H.-R., see S. Koppe 214 (1993) 546
Volpp, H.-R., see A. Jacobs 218 (1994) 51
Von Helden, G., N.G. Gotts and M.T. Bowers, C_7^+ is cyclic: experimental evidence 212 (1993) 241
Von Helden, G., W.E. Palke and M.T. Bowers, The lowest energy structures of C_7^+, C_7 and C_7^-. An ab initio study 212 (1993) 247
Von Niessen, W., see J. Mai 211 (1993) 197
Von Schnering, H.G., see K. Kamarás 214 (1993) 338
Von Schütz, J.U., see A. Angerhofer 217 (1994) 403
Vučković, M., see I. Gutman 216 (1993) 447

Wachter, W., see C. Berg 216 (1993) 465
Waclawik, E.R., see R.A.J. Borg 218 (1994) 320
Wahnon, P., see B. Ramiro Diaz 212 (1993) 218
Wakabayashi, T., see K. Kikuchi 216 (1993) 67
Wakasa, M., Y. Nakamura, Y. Sakaguchi and H. Hayashi, Magnetic field effects on hydrogen abstraction of triplet xanthone with *p*-aminothiophenol in an SDS micellar solution 215 (1993) 631
Wakoh, K., see Y. Saito 212 (1993) 379
Walch, S.P., Characterization of the potential energy surface for $CH_3+O_2\rightarrow$products 215 (1993) 81
Waldman, A. and S. Ruhman, A femtosecond time-resolved transient bleach study of the benzene excimer 215 (1993) 470
Wales, D.J., Ab initio calculation of molecular structure by expansion of the electron density 217 (1994) 302
Wales, D.J., see R.M. Minyaev 218 (1994) 413
Walker, M.B., see D.F. Agterberg 213 (1993) 207
Wall, M.C., see J.L. Tomer 216 (1993) 286
Wallington, T.J., M.D. Hurley, J.C. Ball and M.E. Jenkin, FTIR product study of the reaction of $CH_3OCH_2O_2+HO_2$ 211 (1993) 41
Wallington, T.J., M.D. Hurley and W.F. Schneider, Kinetic study of the reaction $CF_3O+O_3\rightarrow CF_3O_2+O_2$ 213 (1993) 442
Wallington, T.J., see J. Sehested 213 (1993) 457
Wallington, T.J., M.D. Hurley, W.F. Schneider, J. Sehested and O.J. Nielsen, Mechanistic study of the gas-phase reaction of CH_2FO_2 radicals with HO_2 218 (1994) 34
Wallington, T.J., see T. Ellermann 218 (1994) 287
Walther, K.L., U. Krämer, H. Hoffmann and A. Wokaun, Electric birefringence in surfactant and polyelectrolyte solutions. Fourier relations between transient and frequency-dependent measurements 212 (1993) 96
Walton, D.R.M., see H.W. Kroto 214 (1993) 353
Walz, J., K. Ulrich, H. Port, H.C. Wolf, J. Wonner and F. Effenberger, Fulgides as switches for intramolecular energy transfer 213 (1993) 321
Wang, C.Z., see X.Q. Wang 214 (1993) 193; 217 (1994) 199
Wang, H., see X. Zhao 214 (1993) 203
Wang, H., X. Chen and B.R. Weiner, $SO(X\ ^3\Sigma^-)$ production from the 193 nm laser photolysis of thionyl fluoride 216 (1993) 537
Wang, H.X., see A. Takahashi 216 (1993) 394
Wang, J., see L.A. Eriksson 211 (1993) 88
Wang, J. and P. Wolynes, Passage through fluctuating geometrical bottlenecks. The general Gaussian fluctuating case 212 (1993) 427
Wang, J. and V.H. Smith Jr., Evaluation of electron pair densities and their Laplacians in atomic systems 220 (1994) 331
Wang, J.T., see T. Bally 212 (1993) 141
Wang, K., V. McKoy and H. Rudolph, Rotationally resolved photoelectron spectra in (2+1) resonance-enhanced multiphoton ionization of NO via the C $^2\Pi$ Rydberg state 217 (1994) 490
Wang, K., M.-T. Lee, V. McKoy, R.T. Wiedmann and M.G. White, Rotationally resolved threshold photoelectron spectroscopy of H_2O and H_2S 219 (1994) 397
Wang, L.-M., see A.S. Gurav 218 (1994) 304
Wang, P., see L. Xu 212 (1993) 265
Wang, S., see S. Seraphin 217 (1994) 191
Wang, X., see Q. Zhu 212 (1993) 403

Wang, X.-D., T. Hashizume, Q. Xue, H. Shinohara, Y. Saito, Y. Nishina and T. Sakurai, Geometry of metallofullerenes adsorbed on the Si(100)2×1 surface studied by scanning tunneling microscopy 216 (1993) 409
Wang, X.Q., C.Z. Wang, B.L. Zhang and K.M. Ho, First-principles study of C_{96} fullerene isomers 214 (1993) 193
Wang, X.Q., C.Z. Wang, B.L. Zhang and K.M. Ho, Electronic structures of C_{82} fullerene isomers 217 (1994) 199
Wang, X.-Y., see Z.-L. Cai 213 (1993) 168
Wang, Y., J.M. Holden, Z.-H. Dong, X.-X. Bi and P.C. Eklund, Photo-dimerization kinetics in solid C_{60} films 211 (1993) 341
Wang, Y., see L. Xu 212 (1993) 265
Wang, Y., C.A. Woodward and W.A. Chupka, Ionic state preparation of O_2^+ via the 3dδ $^{1,3}\Phi_g$ Rydberg states of O_2 214 (1993) 290
Wang, Y., J.M. Holden, X. Bi and P.C. Eklund, Thermal decomposition of polymeric C_{60} 217 (1994) 413
Wang, Y., see J.V. Caspar 218 (1994) 221
Wang, Y. and C.X.W. Qian, The role of fragment rotation in the femtosecond dissociation of ICN 219 (1994) 389
Wannous, G., see R.F. Barrow 214 (1993) 293
Warken, M., see C. Schmidt 211 (1993) 272
Warken, M., see K. Dietz 220 (1994) 397
Washida, N., see A. Masaki 218 (1994) 523
Watanabe, J., H. Takahashi, J. Nakahara and T. Kushida, Subpicosecond dynamic Stokes shift in β-carotene solution probed by excitation energy dependence of fluorescence spectrum 213 (1993) 351
Watanabe, K., see K. Hoshino 211 (1993) 571
Watanabe, K., see A. Nakajima 214 (1993) 22
Weaver, M.J., see C. Stuhlmann 219 (1994) 319
Weber, P.M., see N. Thantu 214 (1993) 276
Wehrum, G., see G. Blasse 215 (1993) 363
Wei, S., see S.F. Cartier 220 (1994) 23
Weiner, B.R., see X. Gu 211 (1993) 65
Weiner, B.R., see H. Wang 216 (1993) 537
Weiss, R., see T.-H. Tran-Thi 213 (1993) 139
Weiss, S., Uniform reduced interaction dipole for all rare gas pairs revisited 219 (1994) 339
Weitz, E., see D. LaBrake 211 (1993) 430
Weitz, E., see S.J. Garrett 219 (1994) 409
Wells, B.O., see C.-H. Park 213 (1993) 196
Weltner Jr., W., see R.J. Van Zee 217 (1994) 381
Werner, H.-J., see A. Spielfiedel 216 (1993) 162
Werner, H.-J., see M. Baer 219 (1994) 372
Werst, D.W., see K.R. Cromack 218 (1994) 485
Wertheim, G.K., see J.M. Gildemeister 220 (1994) 181
West, D.S., see D.A. Dolson 216 (1993) 258
West, Y.D., see A. Carrington 212 (1993) 473
Westh, P., A. Hvidt and Y. Koga, Transition of the mixing scheme in the water-rich region of aqueous 2-butoxyethanol: heat capacities and their temperature derivatives 217 (1994) 245
Wheeler, M.D., I.R. Lambert and M.N.R. Ashfold, Two-colour laser-induced grating spectroscopy of iodine vapour 211 (1993) 381

Whetten, R.L., see K. Hansen 218 (1994) 462
White, J.A. and D.M. Bird, Dissociative adsorption of H_2 on Cu(100) 213 (1993) 422
White, J.M., see Z.-J. Sun 219 (1994) 118
White, M.G., see K. Wang 219 (1994) 397
Whyman, G.E., see M.M. Mestechkin 214 (1993) 144
Wick, M.T., B. Nickel and A.A. Ruth, The $S_0 \rightarrow S_3$ transition in 1,2-benzanthracene. Experimental evidence for the statistical limit of vibronic coupling of S_3 with S_2 215 (1993) 243
Widmann, D., see A. Angerhofer 217 (1994) 403
Wiedmann, R.T., see K. Wang 219 (1994) 397
Wieme, W., see L. Goubert 219 (1994) 360
Wiering, P.G., see S.I. van Dijk 214 (1993) 502
Wiersma, D.A., see E. Lenderink 211 (1993) 503; 218 (1994) 586
Wild, U.P., see M. Croci 212 (1993) 71
Wild, U.P., see F. Güttler 217 (1994) 393
Wilhelm, J., see G. Colonna 213 (1993) 5
Willey, K.F., C.S. Yeh and M.A. Duncan, Mass-analyzed threshold ionization spectroscopy of Al–Ar 211 (1993) 156
Williams, D.E., see Y. Xiao 215 (1993) 17
Williams, E.D., see B. Li 217 (1994) 595
Williams, F., see T. Bally 212 (1993) 141
Williams, I.H., see J.S. Francisco 214 (1993) 591
Williams, R., see K. Ravichandran 217 (1994) 375
Williams, S., see R.A. Dressler 215 (1993) 656
Williamson, J.C., see Ch. Lienau 213 (1993) 289
Wilson, G.J., M.L. Turnidge and C.J.S.M. Simpson, The vibrational deactivation of $^{12}C^{16}O$ by H_2 and D_2 in liquid D_2 solution 214 (1993) 297
Windus, T.L., M.W. Schmidt and M.S. Gordon, Parallel algorithm for SCF analytic Hessians. I. Small scale algorithm 216 (1993) 375
Wine, P.H., see R.E. Stickel 212 (1993) 312
Winkler, D.C., J.H. Moore and J.A. Tossell, Inner-shell electron excitation in the chlorosilanes 219 (1994) 57
Winkler, R., see G. Colonna 213 (1993) 5
Winnik, M.A., see A.T. Reis e Sousa 213 (1993) 333
Winstead, C., see J.F. Ying 212 (1993) 289
Wirz, J., see M. Mac 211 (1993) 20
Wiskerke, A.E., C.A. Taatjes, A.W. Kleyn, R.J.W.E. Lahaye, S. Stolte, D.K. Bronnikov and B.E. Hayden, Survival mechanism for rotational rainbows in highly attractive molecule–surface systems: NO scattering from Pt(111) 216 (1993) 93
Withers, J.C., see S. Seraphin 217 (1994) 191
Wittig, C., see H.F. Davis 215 (1993) 214
Wodtke, A.M., see G. Meijer 217 (1994) 112
Wokaun, A., see K.L. Walther 212 (1993) 96
Wolf, H.C., see J. Walz 213 (1993) 321
Wolf, I., see H. Ernst 212 (1993) 588
Wolf, J.P., see K. Kobe 213 (1993) 554
Wolfrum, J., see S. Koppe 214 (1993) 546
Wolfrum, J., see A. Jacobs 218 (1994) 51

Wolfrum, K., H. Graener and A. Laubereau, Sum-frequency vibrational spectroscopy at the liquid–air interface of methanol. Water solutions 213 (1993) 41
Wöll, Ch., see Ch. Zubrägel 219 (1994) 127
Wolynes, P., see J. Wang 212 (1993) 427
Wolynes, P.G., see S.A. Schofield 217 (1994) 497
Wong, A.T. and G.B. Bacskay, Ab initio prediction of the vibrational frequencies of N_2S 217 (1994) 17
Wong, C.M., see I.Y. Chan 219 (1994) 187
Wong, S.S., see N.L. Ma 213 (1993) 189
Wonner, J., see J. Walz 213 (1993) 321
Woo, S.I., see I.J. Park 212 (1993) 505
Woodward, C.A., see Y. Wang 214 (1993) 290
Wormer, P.E.S., see G. Jansen 214 (1993) 103
Worthington, S.E., see C.J. Cramer 218 (1994) 387
Wöste, L., see K. Kobe 213 (1993) 554
Woywod, C., see W. Domcke 216 (1993) 362
Woźniak, K., see S.T. Howard 212 (1993) 1
Wozniak-Braszak, A., see E.C. Reynhardt 215 (1993) 493
Wright, J.S., see M. Kolbuszewski 218 (1994) 338
Wu, J., see R. Huang 216 (1993) 108, 115
Wu, R., see C. Halvorson 212 (1993) 85
Wu, X., B. Ramachandran and R.E. Wyatt, A single arrangement variational method for total reaction probabilities 214 (1993) 118
Wu, X., see A.S. Jeevarajan 219 (1994) 427
Wu, Y.-S.M., see A. Kuppermann 213 (1993) 636
Wudl, F., see C. Halvorson 212 (1993) 85
Wurfel, B.E., see N. Caspary 212 (1993) 329
Wurfel, B.E., see G. Schallmoser 219 (1994) 101
Wyatt, R.E., see X. Wu 214 (1993) 118
Wyatt, R.E., see L.J. Brenner 215 (1993) 63

Xiao, Y. and D.E. Williams, Genetic algorithm: a new approach to the prediction of the structure of molecular clusters 215 (1993) 17
Xu, C., see D.L. Strout 214 (1993) 576
Xu, D., see G. Ding 220 (1994) 1
Xu, H., see N.E. Shafer 212 (1993) 155
Xu, J., see L.D. Hulett Jr. 216 (1993) 236
Xu, L., Y. Wang, P. Wang and F. Li, High-resolution (2+1) multiphoton ionization spectroscopy of Br_2 212 (1993) 265
Xu, S., Y.J. Kim and J. Jonas, Pressure effects on the anisotropic rotational diffusion of acetonitrile-d_3 in confined geometry 218 (1994) 329
Xu, Z., see M. Neeb 212 (1993) 205
Xue, Q., see X.-D. Wang 216 (1993) 409

Yadav, T., see S. Seraphin 217 (1994) 191
Yagi, M., I. Itoh, A. Komura, K. Hayashi and J. Higuchi, A time-resolved EPR study of the triplet states of 4-phenylpyridine and its protonated cation and of biphenyl 211 (1993) 179
Yamabe, T., see Y. Matsuzaki 211 (1993) 300
Yamabe, T., see K. Yoshizawa 213 (1993) 498
Yamabe, T., see K. Okahara 219 (1994) 462
Yamaguchi, K., see M. Okumura 219 (1994) 36
Yamamoto, K., see T. Miyazaki 219 (1994) 405
Yamamoto, S., The microwave spectrum of SO in the b $^1\Sigma^+$ electronic state 212 (1993) 113
Yamamoto, S., H. Mizuma, A. Nitta, N. Fukazawa, H. Fukumura and H. Masuhara, The initial photochemical process of triosmiumdodecacarbonyl adsorbed on the surface of silica as studied by picosecond diffuse reflectance laser photolysis and matrix isolation 215 (1993) 323
Yamamuro, S., see Y. Saito 212 (1993) 379
Yamani, Z.H., see U.K.A. Klein 217 (1994) 80
Yamano, Y., see M. Mimuro 213 (1993) 576
Yamasaki, K., A. Tanaka, I. Tokue and Y. Ito, Spin-forbidden excitation of $CF_2(\tilde{a}\ ^3B_1 \leftarrow \tilde{X}\ ^1A_1)$ by collisions with $N_2(A\ ^3\Sigma_u^+)$ 215 (1993) 483
Yamashita, M., see N. Kimura 220 (1994) 40
Yamato, T., M. Saito and J. Higo, Topographical metric to analyze the thermal fluctuations of protein conformation 219 (1994) 155
Yamazaki, I., see M. Mimuro 213 (1993) 576
Yáñez, M., see O. Mó 219 (1994) 45
Yang, D.Y., see B. Fain 216 (1993) 551
Yang, J., see C.G. Joslin 211 (1993) 587; 213 (1993) 377; 215 (1993) 144
Yang, J., see W. Głaz 218 (1994) 183
Yang, S.I., see E. Shin 218 (1994) 107
Yang, T.-S., see R. Zhang 211 (1993) 541
Yang, W., see G. Ding 220 (1994) 1
Yang, X., C.J. Petrillo and C. Noda, Photoacoustic detection of N_2O and CO_2 overtone transitions in the near-infrared 214 (1993) 536
Yang, X., see P. Felder 215 (1993) 221
Yang, Y., see R. Liyanage 216 (1993) 544
Yannoni, C.S., see C.-H. Park 213 (1993) 196
Yannouleas, C. and U. Landman, Stabilized-jellium description of neutral and multiply charged fullerenes $C_{60}^{x\pm}$ 217 (1994) 175
Yartsev, A.P., see I.V. Bezel 218 (1994) 475
Yashonath, S., see A. Chakrabarti 215 (1993) 591
Yasui, Y., see T. Takaoka 215 (1993) 523
Ye, C., see X. Mao 218 (1994) 249
Yeates, A.T., see G.P. Das 212 (1993) 671
Yeh, C.S., see K.F. Willey 211 (1993) 156
Yen, W.M., see H. Eilers 212 (1993) 109
Yen, W.M., see U. Hömmerich 213 (1993) 163
Yeretzian, C., see K. Hansen 218 (1994) 462
Yeung, M.T., see K.A. McLauchlan 217 (1994) 157
Yin, H.-M., see Z.-X. Ma 213 (1993) 250

Ying, J.F., C.P. Mathers, K.T. Leung, H.P. Pritchard, C. Winstead and V. McKoy, Observation of a "new" quadrupole transition at 7.7 eV in CF_3Cl by momentum-transfer-resolved electron energy loss spectroscopy 212 (1993) 289
Ying, Q., J. Marecek and B. Chu, Slow aggregation of buckminsterfullerene (C_{60}) in benzene solution 219 (1994) 214
Yodh, A.G., see J.P. Culver 214 (1993) 431
Yokoyama, Y., see J. Takeda 220 (1994) 443
Yorish, V.S., The partition function of free internal rotation. Combined direct and transformed expressions numerical study 219 (1994) 279
Yoshihara, K., see R. Inaba 211 (1993) 183
Yoshihara, K., see H. Kandori 211 (1993) 385
Yoshihara, K., see A.E. Johnson 211 (1993) 511
Yoshihara, K., see B. Kim 212 (1993) 271
Yoshihara, K., see P.B. Bisht 213 (1993) 75
Yoshihara, K., see V.F. Kamalov 213 (1993) 559; 220 (1994) 257
Yoshihara, K., see H. Sekiya 215 (1993) 641
Yoshihara, K., see A. Douhal 217 (1994) 619
Yoshikawa, K., T. Kusumi, M. Ukitsu and S. Nakata, Generation of periodic force with oscillating chemical reaction 211 (1993) 211
Yoshikawa, T., see Y. Saito 212 (1993) 379
Yoshinobu, J., N. Takagi and M. Kawai, Site conversion of CO on Ni(100): binding-energy difference and role of low-energy hindered vibrations 211 (1993) 48
Yoshinobu, J., see N. Takagi 215 (1993) 120
Yoshizawa, K., T. Sato, K. Tanaka, T. Yamabe and K. Okahara, ESR study of TDAE–C_{60} and TDAE–C_{70} in solution 213 (1993) 498
You, W.-M., see S. Qin 213 (1993) 373
Young, M.A., see L.N. Ding 212 (1993) 499
Young, P.E. and I.H. Hillier, Hydration free energies of nucleic acid bases using an ab initio continuum model 215 (1993) 405
Young, P.E., see R.J. Hall 220 (1994) 129
Yoxall, K.R., see D.M. Smith 216 (1993) 493
Yu, D.H., see L.H. Andersen 217 (1994) 204

Zadkov, V.N., see V.D. Vachev 215 (1993) 306
Zadoyan, R., Z. Li, P. Ashjian, C.C. Martens and V.A. Apkarian, Femtosecond dynamics of coherent photodissociation–recombination of I_2 isolated in matrix Ar 218 (1994) 504
Zahradník, R., see P. Jungwirth 212 (1993) 211; 217 (1994) 319
Zaitsevskii, A.V., see V.I. Alexandrov 218 (1994) 206
Zakhidov, A., see F. Negri 211 (1993) 353
Zamboni, R., see O. Dippel 216 (1993) 418
Zamboni, R., see F. Kajzar 217 (1994) 418
Zanasi, R., see P. Lazzeretti 220 (1994) 299
Zanazzi, E., see C. Comicioli 214 (1993) 438
Zapadinsky, E.L., see B.Z. Gorbunov 215 (1993) 31
Zare, R.N., see N.E. Shafer 212 (1993) 155
Zare, R.N., see W.R. Simpson 212 (1993) 163
Zarubaiko, A.M., see J.V. Gilbert 220 (1994) 19
Zeaiter, H.A., see M. Castillejo 214 (1993) 227
Zecca, A., see G. Karwasz 211 (1993) 529
Zehnacker-Rentien, A., see F. Lahmani 220 (1994) 235
Zeitler, E., see B. Rausenberger 215 (1993) 109
Zekovic, Lj.D., see B.R. Jovanic 216 (1993) 47
Zellner, R., see Ch. Fockenberg 218 (1994) 21
Zerbetto, F., see F. Negri 211 (1993) 353
Zerbi, G., see M. Nisoli 220 (1994) 64
Zerne, R., see P. Erman 215 (1993) 173
Zewail, A.H., see Ch. Lienau 213 (1993) 289
Zewail, A.H., see M.H.M. Janssen 214 (1993) 281
Zhai, R., see Z. Song 217 (1994) 142
Zhang, B., see K. Raghavachari 220 (1994) 385
Zhang, B.L., see X.Q. Wang 214 (1993) 193; 217 (1994) 199
Zhang, C., see W. Sun 218 (1994) 515
Zhang, F. and M.A. Collins, Effective interchain interactions and twiston models in crystalline polyethylene 214 (1993) 459
Zhang, J.Z., R.H. O'Neil, T.W. Roberti, J.L. McGowen and J.E. Evans, Femtosecond studies of trapped electrons at the liquid–solid interface of aqueous CdS colloids 218 (1994) 479
Zhang, Q.-E., see W.-D. Cheng 216 (1993) 353
Zhang, R., T.-S. Yang and A.B. Myers, Femtosecond incoherent photon echo from rhodamine B in propylene glycol. Inhomogeneous broadening and spectral diffusion at room temperature 211 (1993) 541
Zhang, R.-P., see A. Osuka 215 (1993) 179
Zhang, X.-G., see Z.-L. Cai 213 (1993) 168
Zhang, Y., see E.I. Haskal 219 (1994) 325
Zhao, X., S. Ong, H. Wang and K.B. Eisenthal, New method for determination of surface pK_a using second harmonic generation 214 (1993) 203
Zhao, Z., see R.E. Stickel 212 (1993) 312
Zharikov, A.A. and P.A. Frantsuzov, Non-adiabatic and adiabatic regimes of transitions between intersecting terms. Applications to electron transfer 220 (1994) 319
Zheludev, N.I., see A.R. Bungay 217 (1994) 249
Zheng, Y.C. and J. Almlöf, Density functionals without meshes and grids 214 (1993) 397

Zhiwu, P., see G. Blasse 215 (1993) 363
Zhou, D., see S. Seraphin 217 (1994) 191
Zhou, P., Z.-H. Dong, A.M. Rao and P.C. Eklund, Reaction mechanism for the photopolymerization of solid fullerene C_{60} 211 (1993) 337
Zhou, P., see J.M. Holden 220 (1994) 186
Zhou, X., see R. Liu 212 (1993) 702
Zhu, P.W., Viscosity study of oligomer-induced coil–globule transition of a polystyrene 215 (1993) 627
Zhu, Q., H. Li and X. Wang, Anharmonicity: a route to vibrational localization 212 (1993) 403
Zhu, W., see Y. Huang 213 (1993) 209; 214 (1993) 451
Zhu, W., Y. Huang, D.J. Kouri, C. Chandler and D.K. Hoffman, Orthogonal polynomial expansion of the spectral density operator and the calculation of bound state energies and eigenfunctions 217 (1994) 73
Zhu, W., see D.J. Kouri 220 (1994) 312
Zidan, M.D., see C.M. Quintella 214 (1993) 563
Zieger, G., see R. Konrat 212 (1993) 78
Ziegler, C., see P. Lemoine 220 (1994) 177
Ziesel, J.-P., see R. Azria 220 (1994) 417
Zimont, E.V., see A.A. Iogansen 212 (1993) 604
Zitserman, V.Yu., see A.M. Berezhkovskii 212 (1993) 413
Zorinyants, G.E., see M.M. Triebel 214 (1993) 315, 321
Zotti, G., see M. Nisoli 220 (1994) 64
Zubrägel, Ch., F. Schneider, M. Neumann, G. Hähner, Ch. Wöll and M. Grunze, Electronic structure of alkane chains. Complete one-dimensional band structures of the valence states 219 (1994) 127
Zumofen, G. and J. Klafter, Spectral random walk of a single molecule 219 (1994) 303
Zumwalt, M.C., see L. Nemes 218 (1994) 295
Zupan, A., see M. Causà 220 (1994) 145
Zurita, S., see J. Rubio 217 (1994) 283
Zyss, J., see J.-M. Nunzi 219 (1994) 349

Mössbauer Studies of Surface Layers

By **G.N. Belozerski**

Studies in Physical and Theoretical Chemistry Volume 81

Mössbauer spectroscopy has evolved as one of the few methods available for investigation of solids differing in depth by several orders of magnitude. This recent development has made the problems of surface investigation and the study of separate layers amenable to investigation. The parameters of the hyperfine interaction derived from the Mössbauer spectra provide valuable information on the chemical bond character and on magnetic properties of surface layers as well as on the change of the properties with the depth from the outermost surface layer. It is possible to carry out quantitative phase analysis and to use the technique to study different transformations in the solid which result from external effects under a wide range of temperatures and pressures.

This book is one of the first attempts at a consistent presentation of theoretical and practical problems of the use of Mössbauer spectroscopy to study solid surfaces, its applications, and development. The applications include: surface studies with hyperfine probes in the following fields: oxidation and corrosion of metals and alloys: passivating and protective coatings: physics of metals: annealing and quenching, mechanical and chemical treatment, ion implantation and laser treatment; texture of near-surface layers. Mössbauer spectroscopy is one of the best methods for *in situ* characterization of solid/solid and solid/solution interfaces. It lends itself to *in situ* studies of surfaces under various coatings and processes, surface magnetism and the effect of the gas phase on the properties of the surface layers and the structure and magnetic properties of epitaxially grown monolayers on the surface of oriented single crystals.

Contents: Preface. **1. Physical Concepts of the Method.** General Aspects of Mössbauer Spectroscopy. Hyperfine Interactions and Line Positions in Mössbauer Spectra. Relative Intensities of Spectral Lines. Experimental. References. **2. Mössbauer Spectroscopy Based on Detection of Electromagnetic Radiation.** Radiation Transmission through Matter. Low-Energy γ-Quanta Scattering. Resonance Fluorescence and Interference Effects. Angular Dependencies of the Scattered γ-Radiation. Mössbauer γ-Quanta Scattering as a Method of Surface Study. Scattering Experiments with Detection of Characteristic X-rays. A Theory of Backscattering Mössbauer Spectroscopy (X-Rays Detection). Backscattering Mössbauer Spectroscopy by the Detection of X- and γ-Radiation. Practical Aspects. References. **3. Mössbauer Spectroscopy Based on the Detection of Electrons.** The Interaction of Electrons with Matter Following Mössbauer Scattering. Conversion Electron Mössbauer Spectroscopy Theory Based on the Exponential Attenuation of the Electron Beam. Theory of CEMS Based on Elementary Electron Interactions. Depth Selective Conversion Electron Mössbauer Spectroscopy. β-Spectra and Weight Functions for DCEMS. Structure Determination of Near Surface Layers by DCEMS. Proportional Counters as Electron Detectors in CEMS. Depth Selection by Means of Proportional Counters. Analysis of Thin Layers under Total External Reflection of Mössbauer Radiation. Other Methods of Detection in CEMS. Channeltrons and the Detection of Very-Low Energy Electrons. References. **4. Mössbauer Backscattering Spectra.** Weight Functions and Re-scattering. Evaluation of the Intensity of Scattered γ-Radiation. Evaluation of the Intensity of X-Rays and Electrons. Line Shapes and Intensity Ratios. The Quality of a Mössbauer Spectrum. Quantitative Information from Mössbauer Spectra. Layer-by-Layer Analysis. References. **5. Practical Aspects of Surface Layer Analysis.** Corrosion Studies of Metals and Alloys. Applications in Metal Physics. Ion Implantation and Laser Treatment of Metals. Spin Texture Studies of Surface Layers. Some Other Applications. References. Variables and Abbreviations (alphabetic). **Index.**

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Inorganic Polymeric Glasses

By **R.C. Ropp**, *Warren, NJ, USA*

Studies in Inorganic Chemistry Volume 15

The author describes a novel method of preparing hydrolysis-stable non-silicate glasses which is based on experimental work accomplished over the past twenty years. As such, the method is the beginning of a new approach to glass-making by the use of a molecularly-polymerizable precursor.

The book elucidates the technical details required to produce such molecularly-polymerized glasses from carefully prepared inorganic molecular monomers. Essentially, only silicate-based glasses have been known to be stable, whereas non-silicate glasses could not be attributed with such properties. Such glasses have, therefore, not found widespread usage in industry. The new phosphate glasses described here exhibit stabilities superior to many of the silicate glasses.

Researchers in glass and glass properties will find this volume extremely useful and those involved in organic polymers will be intrigued by the similarities and disparities of the two systems.

Contents: 1. Introduction to Silicate Glass Technology.
Glass and Antiquity. The Glassy or Vitreous State. Glass Formers and Glass Compositions. The Manufacture of Silicate-Based Glasses. Forming and Finishing Operations. Thermal Processing and Properties of Silicate Glasses. Inherent Properties of Glass. Silicate Glass Products Currently being Manufactured.
2. Introduction to Polymeric Glasses.
Prior Attempts to Prepare Stable Phosphate Glasses. Structural Units in Glass. Basis for Chain Structure of Polymerized Phosphates. Prior Attempts to Prepare Phosphate Glasses by the Melting of Stoichiometric Compounds. Crystalline Salt Monomers for Stable Phosphate Glass Preparation.
3. Factors Contributing to the Preparation of Stable Phosphate Glasses.
Anomalous Recrystallization of Polymeric Calcium Phosphate Glass. Abnormal Strain Relief Behavior of Polymeric $[Ca(PO_3)_2]_n$ Glass. The Effect of Melt Hold Time on Glass Points. Measurement of Hydrolysis Stability of Polymerized Glasses. Effects of Purity and Melt Hold Time on Hydrolysis Stability of Polymerized Glasses. Effect of Melt Hold Time on Melt Viscosity. Effect of Excess H_3PO_4 on the Reaction Paths of Monobasic Salts. Effect of Ca/P Ratios on Stability of Polymerized Glass Compositions. Other Polymerized Alkaline Earth Phosphate Glasses. Effect of Crucibles Used to Hold the Melt during Polymerization. The Combined Effects of Purity and MHT upon Polymerization.
4. Further Aspects of Polymerized Phosphate Glasses.
The Impurity Phase-Segregation Phenomenon. Phase Separation as a Function of *"M"* in $[CaM(PO_3)_2]_n$ Glass. Physical Properties of Fully Polymerized Phosphate Glasses. Elimination of Striae and Other Optical Defects. Spectral Properties and Ultraviolet Transparency. Internal Diffusion Mechanisms and Modes of Chemical Attack. Optimal Methods of Purification. Other Inorganic Polymeric Glasses.
5. Uses of Polymeric Phosphate Glasses.
Nuclear Waste Sources. History of Glass as a Nuclear Waste Encapsulent. Polymeric Phosphate Glass and Nuclear Waste Encapsulation. Properties of a Polymeric Phosphate Glass Containing Nuclear Waste. Luminescent Polymeric Phosphate Glass and its Applications. Other Potential Uses of Polymeric Glass.
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Dynamics of Excited Molecules

Edited by **Kozo Kuchitsu**

Studies in Physical and Theoretical Chemistry Volume 82

The physical and chemical properties of the molecular species reviewed in this book, and sometimes the species themselves, had been postulated or predicted but their exact details remained essentially unexplored for decades. The recent advances in chemical physics (such as laser spectroscopy and quantum-theoretical calculations) have provided techniques for their unambiguous identification. Accurate data on their structures and dynamics are now available. Such information is indispensable for detailed discussion on the various properties of molecules and the mechanisms of intermolecular interactions and chemical interactions.

Information on the dynamics of excited molecules constitutes a firm basis of modern chemistry and physics. Moreover, it is of paramount importance in various fields of basic and applied sciences where chemical reactions play important roles: atomic and molecular physics, atmospheric and environmental science, space science, materials science, and biology.

This book contains 13 review articles on
(1) the techniques for production and identification of excited molecules in the gas phase, condensed phases, and intermediate phases (intermolecular complexes and atomic or molecular microclusters)
(2) their structures and dynamics (internal reactions) observed mainly by spectroscopic experiments
(3) their important roles in chemical processes. The target chemical species range from diatomics to relatively complicated aromatics in a variety of electronic and vibrational excited states, many of them being nonrigid or short-lived molecules, radicals, and positive or negative ions.

Contents:

1. Dynamics of excited molecules. An introduction (K. Kuchitsu, S. Tsuchiya).
2. Infrared diode laser and microwave kinetic spectroscopy (H. Kanamori *et al.*).
3. Free jet infrared spectroscopy of weakly bound complexes (M. Takami *et al.*).
4. Large-amplitude motions of aromatic molecules as studied by supersonic jet spectroscopy (M. Ito).
5. Decay processes of inner-shell photoexcited molecules (Y. Sato)
6. Dynamics of superexcited molecules (Y. Hatano).
7. Vibrational dynamics in highly excited polyatomic molecules (K. Yamanouchi, S. Tsuchiya).
8. Dynamics of ion-molecule reactions (I. Koyano).
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by **N.M. van Os, J.R. Haak** *and* **L.A.M. Rupert**

The number of physico-chemical investigations of surfactants in solution, whether aqueous or nonaqueous, has dramatically increased in recent years. However, literature reports on surfactants in solutions are scattered over a plethora of scientific journals and books which differ widely in scope and readership. Such data are often difficult to retrieve because there have been no systematic compilations, with the exception of those for CMCs and for micelle aggregation numbers.

The present compilation meets that need by covering, as completely as possible, the physico-chemical properties of selected series of homologous surfactants. These surfactants are in most cases isomerically pure, are well-known, and have been used in numerous academic and industrial studies. The properties include aggregation number, cloud point, CMC, ^{13}C-NMR, correlation length, counterion binding, density, enthalpy of micelle formation, entropy of micelle formation, Gibbs' free energy of micelle formation, head group area, ^{1}H-NMR, hydration number, Krafft temperature, melting point, micelle radius, microscopic viscosity, miscibility curve, partial molar volume, phase inversion temperature, refractive index, self- diffusion coefficient, surface tension, and upper critical temperature. The book also contains two- and three-component phase diagrams of many nonionic surfactants.

The solvent is water in most cases; however, some data refer to properties in D_2O, electrolyte solutions, and nonaqueous solvents. The variables are temperature and concentration. Where possible, the method of measurement is given. Data on the purity of the compounds and the accuracy of the measurement methods are not included, as these can easily be found in the original sources, which mostly date from the period 1970-1991 and are given at the end of each chapter. The Index section contains a compound index, a property index, a symbol index and a cross index which facilitate easy access to the data.

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